| Seq No | Term | Variable | Description | Cat1\|Cat2\|... | Freq |
|---|---|---|---|---|---|
| 1 | -update gpu | The velocities of the center of mass are now removed correctly in case of -update gpu | A fix for incorrect COM velocity removal when using GPU update | software | 7 |
| 2 | .gitlab-ci.yml | .gitlab-ci.yml | The main configuration file for GitLab CI/CD pipelines | data format | 3 |
| 3 | pdo file | .pdo | An old file format for WHAM output, no longer readable | data format | 0 |
| 4 | 2D/3D dynamic load balancing | Fix error with 2D/3D dynamic load balancing | A fix for an error in dynamic load balancing with a limited cell size | software | 1 |
| 5 | 32bit support | 32bit support | Support for compiling GROMACS as a 32-bit application, which has been removed | software | 2 |
| 6 | AdaptiveCpp | AdaptiveCpp | An open-source SYCL implementation for various hardware platforms | software | 38 |
| 7 | addtogroup | \addtogroup | A Doxygen command to add a block of items to a documentation group | software | 17 |
| 8 | AMBER | AMBER | A set of force fields and a molecular simulation program package | model\|software | 39 |
| 9 | AMD Zen 2 detection | Added AMD Zen 2 detection | A feature to detect this CPU architecture and use tuned non-bonded kernels | software | 1 |
| 10 | Anisotropic temperature factors | anisotropic temperature factors | Factors (Uij) describing atomic displacement in an anisotropic manner | measure | 3 |
| 11 | ARMv7 | ARMv7 | A 32-bit ARM architecture, a deprecated platform | software | 10 |
| 12 | Atom renaming database | arn | A database used to rename atoms to match force field conventions | data source\|data format | 2 |
| 13 | Autocorrelation function | ACF | A function that measures the correlation of a property with itself at different time intervals | measure | 33 |
| 14 | AVX 512 detection code | Fix error in AVX 512 detection code | A fix for a typo in the CMake detection code for AVX-512 | software | 1 |
| 15 | Accelerated Weight Histogram | AWH | An adaptive biasing method to calculate potentials of mean force | algorithm\|method | 16 |
| 16 | AWH FEP dimension | AWH FEP dimension | A bug in grompp checks for AWH settings when sampling a free-energy dimension was fixed | method | 0 |
| 17 | AWH user PMF | AWH user PMF | A feature to provide a user-defined PMF as input to AWH, with a fix for large values | data source | 1 |
| 18 | AWH with pull-geometry 'direction' periodic | Allow AWH with pull-geometry 'direction' to be periodic | A change to make this pull geometry periodic when the AWH interval is large | software | 0 |
| 19 | awh-potential = convolved | awh-potential = convolved | A combination of AWH with a pull dimension that was disabled in grompp due to incorrectness | identifier | 1 |
| 20 | Barostat | c-rescale barostat | An algorithm to control the pressure of a simulation | algorithm\|model | 20 |
| 21 | baseversion-gen.cpp | baseversion-gen.cpp | A generated source file providing version information | data format | 1 |
| 22 | Bennett's Acceptance Ratio (BAR) | Bennett's Acceptance Ratio | A method for calculating free energy differences from two simulations | method\|algorithm | 0 |
| 23 | Berendsen thermostat | berendsen | A thermostat that weakly couples the system to a heat bath | algorithm\|model | 7 |
| 24 | Berendsen coupling | Berendsen coupling algorithms | Thermostat and barostat methods whose use is now further discouraged | method\|algorithm | 2 |
| 25 | Boltzmann inversion | Bolzmann inverting | A method to derive a potential of mean force from a probability distribution | method | 1 |
| 26 | Bonded interactions on CUDA GPU | Bonded interactions are now supported for CUDA GPU offload | A feature to run common bonded and LJ-14 interactions on NVIDIA GPUs with CUDA | method\|software | 0 |
| 27 | Bonded lambdas | bonded-lambdas | The free energy coupling parameter for bonded interactions | measure | 0 |
| 28 | Boost | Boost | A set of C++ libraries, for which the bundled version is now always used | software | 5 |
| 29 | Buckingham potential | Buckingham | A potential model that includes an exponential repulsion term | model | 4 |

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| 30 | buildinfo.h | buildinfo.h | A generated header file containing build environment information | data format | 2 |
| 31 | Bundle muparser | Bundle muparser | GROMACS now bundles the muParser library instead of requiring an external one | software | 1 |
| 32 | C6/C12 parameters | C6/C12 | Alternative parameters for the Lennard-Jones potential | model | 0 |
| 33 | CamelCase | CamelCase | A naming convention where words are joined without spaces, with each word's first letter capitalized | identifier | 2 |
| 34 | Chain separator | chainsep | An option in pdb2gmx to define how to separate chains in a PDB file | software | 0 |
| 35 | Change Management | Change Management | The process and tools used for managing revisions to the source code | process | 11 |
| 36 | CHARMM | CHARMM | A set of force fields and a molecular simulation program package | model\|software | 30 |
| 37 | CHARMM27 | CHARMM27 | An all-atom version of the CHARMM force field, officially supported in GROMACS | model | 6 |
| 38 | check target | check | A build target that builds and runs all tests | software | 2 |
| 39 | check-source target | check-source | A build target that runs static analysis scripts on the source code | software | 4 |
| 40 | checkpoint files out of sync | Fix checkpoint files getting out of sync with simulations sharing data | A fix to add an MPI barrier before renaming checkpoint files to prevent them from getting out of sync | software | 0 |
| 41 | clang-format | clang-format | An automatic source code formatting tool used by GROMACS | software | 43 |
| 42 | clFFT fallback | disabled internal clFFT fallback used for OpenCL support | A fix to issue a fatal error when the bundled clFFT cannot be built with MSVC | software | 1 |
| 43 | CMake toolchain file | gromacs-toolchain.cmake | A file to help configure client builds, which has been replaced by a hints file | data format | 1 |
| 44 | Code Review | Code Review | The process of having other developers review code changes for correctness and quality | process | 8 |
| 45 | Collective variables (Colvars) | colvars-active | A software module for defining and biasing collective variables | software\|method | 4 |
| 46 | COM removal with frozen atoms | Fix center of mass motion removal with frozen atoms | A fix to correctly remove completely frozen atoms from COM removal groups in grompp | software | 0 |
| 47 | Combined bending-torsion potential | combined bending-torsion potential | A potential term that couples angle bending and torsional rotation | model | 3 |
| 48 | completion target | completion | A build target that generates shell command-line completions | software | 0 |
| 49 | Computational Electrophysiology | swapcoords | Simulations of ion channels including ion/water exchanges | method | 12 |
| 50 | cond | \cond | A Doxygen command to conditionally exclude a block of documentation | software | 16 |
| 51 | config.h | config.h | A generated header file containing defines for conditional compilation | data format | 11 |
| 52 | configure_file | configure_file() | A CMake command that generates a file from a template, substituting variables | software | 1 |
| 53 | Connolly surface | Connolly surface | A type of molecular surface representation, also known as the solvent-excluded surface | model | 2 |
| 54 | Constraints | constraints | Methods to fix bond lengths or angles during a simulation | method\|model | 229 |
| 55 | Continuous Integration | CI | The practice of automatically testing code changes as they are integrated | process | 4 |
| 56 | Delta H output with mass lambda's | Correct free-energy Delta H output with mass lambda's | A fix for double counting of perturbed mass contributions in Delta H output for BAR | measure | 0 |
| 57 | Coupling parameter | coupling parameter | A parameter (lambda) that smoothly transforms one Hamiltonian into another | model | 4 |
| 58 | CP2K | CP2K | A quantum chemistry and solid state physics software package | software | 66 |
| 59 | Cromer's method | Cromer's method | A method for calculating atomic scattering factors for X-rays | method | 0 |
| 60 | CUDA 11.0 | CUDA 11.0 supported | A fix to enable building and testing with CUDA 11.0 | software | 3 |
| 61 | CUDA Graphs for GPU-resident Steps | CUDA Graphs for GPU-resident Steps | A new CUDA feature to launch GPU activities as a single graph, offering performance advantages | method\|software | 1 |

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| 62 | cuFFT | cuFFT | NVIDIA's library for Fast Fourier Transforms on CUDA-enabled GPUs | software | 4 |
| 63 | Cumulative number RDF | cumulative number RDF | The integral of the RDF, representing the average number of particles within a distance r | measure | 1 |
| 64 | Neighbor searching | cutoff-scheme | The method used to generate a list of neighboring atoms | algorithm\|method | 12 |
| 65 | Cygwin | Cygwin | A POSIX-like environment for Windows, for which a compilation issue was fixed | software | 3 |
| 66 | Debye formula | Debye formula | A formula to calculate scattering intensity from a set of atomic coordinates | model | 1 |
| 67 | defgroup | \defgroup | A Doxygen command to define a new documentation group | software | 9 |
| 68 | Demultiplexing | demux | The process of separating a single data stream into its original independent streams | process | 0 |
| 69 | Density-guided simulations | Density-guided simulations | Simulations where forces are applied to fit a structure to a target density map | method\|process | 18 |
| 70 | density-guided-simulation-shift-vector | density-guided-simulation-shift-vector | A new mdp option that defines a shift vector for the density-guided simulation group | identifier | 2 |
| 71 | density-guided-simulation-transformation-matrix | density-guided-simulation-transformation-matrix | A new mdp option that allows defining a matrix to transform structure coordinates | identifier | 4 |
| 72 | dep-graphs target | dep-graphs* | A build target that generates include dependency graphs | software | 1 |
| 73 | Deuterium order parameter | deuterium order parameter | An order parameter (Scd) that can be related to NMR experiments on deuterated lipids | measure | 2 |
| 74 | Development-time tools | Development-time tools | Tools used by developers for tasks like documentation generation and code checking | software | 39 |
| 75 | Diffusion constant | diffusion constant | A measure of the rate of diffusion of a substance | measure | 6 |
| 76 | Dispersion correction | Dispersion correction | Correction applied to energy and pressure for truncated dispersion interactions | method\|model | 14 |
| 77 | Distance matrix | distance matrices | A matrix containing the distances between pairs of residues or atoms | data format | 1 |
| 78 | dlopen | dlopen | A system function to dynamically load shared libraries at runtime | software | 3 |
| 79 | Documentation flavors | Documentation flavors | Different levels of Doxygen documentation generated (e.g., user, lib, full, dev) | identifier | 2 |
| 80 | Documentation generation | Documentation generation | The process of building the GROMACS documentation from various sources | process | 5 |
| 81 | Domain Decomposition | Domain Decomposition | A parallelization strategy that divides the simulation box into spatial domains | algorithm\|method | 126 |
| 82 | Doxygen | Doxygen | A tool for generating documentation from annotated source code | software | 145 |
| 83 | Doxygen groups | Doxygen groups | A Doxygen feature used to organize documentation into logical modules | software | 3 |
| 84 | doxygen-all target | doxygen-all | A build target that generates all flavors of Doxygen documentation | software | 2 |
| 85 | Dynamic selections | dynamic selections | Selections of atoms that can change over the course of a trajectory | method | 6 |
| 86 | Einstein relation for viscosity | Einstein relation | An equation to calculate viscosity from the integral of the pressure tensor autocorrelation function | model\|method | 0 |
| 87 | Electric field | electric-field-x/y/z | An mdp option to apply a time-dependent electric field | identifier | 26 |
| 88 | Ellipticity | Ellipticity | A measure of the circular dichroism signal, often used to characterize helices | measure | 1 |
| 89 | End-to-end distance | end-to-end distance | The distance between the first and last atom of a polymer chain | measure | 2 |
| 90 | Enforced rotation | rotation | Applying a potential to enforce rotation of a group of atoms | method | 11 |
| 91 | Error handling | Error handling | The approach and guidelines for managing runtime errors in GROMACS | process | 10 |
| 92 | Essential Dynamics (ED) | Essential Dynamics (ED) | A method to analyze and sample the large-scale collective motions of a system | method | 1 |
| 93 | Euler rotations | Euler rotations | A method to describe the orientation of a rigid body using three angles | method | 1 |
| 94 | Ewald dipole correction | Ewald dipole correction incorrect without domain decomposition | A fix to disable this correction when not using domain decomposition, as it was incorrect | method | 2 |
| 95 | Ewald summation | Ewald | A method for calculating long-range electrostatic interactions in periodic systems | algorithm\|method | 13 |
| 96 | Expanded ensemble | expanded ensemble | An enhanced sampling method that samples an extended thermodynamic ensemble | method\|algorithm | 48 |

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| 97 | Expanded ensemble restarts | Expanded ensemble simulations restarted from checkpoints | A fix for a bug where restarted expanded ensemble simulations would not run | software | 0 |
| 98 | FEP using AWH | FEP using AWH | A new feature that allows controlling the lambda state of a free energy perturbation with AWH | method | 1 |
| 99 | FEP with modular simulator and DD | Bug fix for FEP calculations with modular simulator and domain decomposition | A fix for incorrect mass handling in FEP calculations with this setup | software | 0 |
| 100 | FFTW | fftw3 | A widely used C subroutine library for computing FFTs | software | 53 |
| 101 | Flooding potential | flooding potential | A biasing potential used in ED sampling to enhance exploration of conformational space | model | 5 |
| 102 | Force Field | Force field | A set of equations and parameters to model molecular interactions | model\|data source | 191 |
| 103 | Fourier Dihedral | Fourier Dihedral | A dihedral potential represented by a Fourier series | model | 2 |
| 104 | g(r) function | g(r) function | The pair correlation function, equivalent to the radial distribution function | measure | 2 |
| 105 | g_membed | g_membed | A GROMACS tool for embedding proteins into membranes, now part of mdrun | software | 5 |
| 106 | Gaussian98 cube format | Gaussian98 cube format | A file format for storing volumetric data, such as electron density | data format | 1 |
| 107 | Generate pairs option | gen-pairs | An option in the topology to automatically generate 1-4 pair interactions | identifier | 0 |
| 108 | Gibbs free energy landscape | Gibbs free energy landscapes | A plot of the Gibbs free energy as a function of one or more collective variables | model | 0 |
| 109 | git commit --amend | git commit --amend | A git command to modify the most recent commit | software | 4 |
| 110 | git commit --fixup | git commit --fixup | A git command to create a commit that will be squashed into an earlier commit | software | 1 |
| 111 | git rebase | git rebase | A git command to re-apply commits on top of another base tip | software | 17 |
| 112 | git stash | git stash | A git command to temporarily store modified tracked files | software | 2 |
| 113 | gitlab | gitlab | The web-based Git repository manager used for GROMACS development | software | 111 |
| 114 | GitLab CI Pipeline | GitLab CI Pipeline | A set of automated jobs for testing and building software in GitLab | process | 1 |
| 115 | GitLab CI Variables | Variables | Environment variables used to control the behavior of GitLab CI jobs and scripts | identifier | 0 |
| 116 | GitLab Container Registry | GitLab Container Registry | A private Docker image registry integrated with GitLab | data source | 3 |
| 117 | GitLab Runner | GitLab Runner | The application that runs jobs in a GitLab CI/CD pipeline | software | 7 |
| 118 | Global templates | Global templates | Reusable job definitions and configuration snippets for GitLab CI | data format | 1 |
| 119 | gmx anadock | gmx anadock | A tool for analyzing AutoDock outputs, which was removed | software | 2 |
| 120 | gmx anaeig | gmx anaeig | A GROMACS tool for analyzing eigenvectors from covariance or normal mode analysis | software | 18 |
| 121 | gmx analyze | gmx analyze | A GROMACS tool for general data analysis of ASCII files | software | 11 |
| 122 | gmx angle | gmx angle | A GROMACS tool to compute and analyze angle distributions | software | 20 |
| 123 | gmx awh | gmx awh | A GROMACS tool to extract and analyze data from AWH simulations | software | 15 |
| 124 | gmx bar | gmx bar | A GROMACS tool for calculating free energy differences using BAR | software | 18 |
| 125 | gmx benchmark | gmx benchmark | A dedicated tool for running performance benchmarks, which now contains certain options previously in mdrun | software | 7 |
| 126 | gmx check | gmx check | A GROMACS tool for checking and comparing various simulation files | software | 16 |
| 127 | gmx chi | gmx chi | An analysis tool for which the deprecation was reverted due to community interest | software | 16 |
| 128 | gmx chi -chi_prod | Fixed gmx chi -chi_prod | A fix for a crash or garbage results when the number of relevant dihedrals differed from the number of residues | software | 1 |
| 129 | gmx chi histogramming | gmx chi histogramming | A fix for a possible crash caused by an invalid reference to a temporary string | software | 1 |

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| 130 | gmx cluster | gmx cluster | A tool for which PDB and index file output was corrected and improved | software | 13 |
| 131 | gmx convert-tpr -s -o | gmx convert-tpr -s -o | A combination of options that was fixed to work with default index groups | software | 1 |
| 132 | gmx convert-tpr -until | gmx convert-tpr -until | A fix for a bug that broke the calculation of remaining steps | software | 1 |
| 133 | gmx covar | gmx covar | An analysis tool for which a range checking bug was fixed | software | 17 |
| 134 | gmx density | gmx density | A tool to calculate density profiles, now always using relative coordinates | software | 12 |
| 135 | gmx densorder | gmx densorder | A GROMACS tool to analyze the interface of a two-phase system | software | 7 |
| 136 | gmx dipoles -quad | gmx dipoles -quad | A fix to make the tool report correct quadrupole values | software | 1 |
| 137 | gmx disre | gmx disre | A tool for which a check for inconsistent distance restraint labels was added | software | 8 |
| 138 | gmx do_dssp | gmx do_dssp | A tool that has been replaced by a native implementation of the DSSP algorithm in gmx dssp | software | 11 |
| 139 | gmx dyndom | gmx dyndom | A tool for analyzing DynDom outputs, which was removed | software | 2 |
| 140 | editconf | gmx editconf | Edits the simulation box and converts structure file formats | software | 34 |
| 141 | gmx genion | gmx genion | A tool for which file permissions of temporary files were fixed | software | 11 |
| 142 | gmx genrestr | gmx genrestr | A GROMACS tool to generate position restraint files | software | 10 |
| 143 | gmx gyrate | gmx gyrate | A GROMACS tool to compute the radius of gyration of a molecule | software | 21 |
| 144 | gmx gyrate-legacy | gmx gyrate-legacy | The old implementation of the gmx gyrate tool | software | 11 |
| 145 | gmx h2order | gmx h2order | A GROMACS tool to compute the orientation of water molecules | software | 8 |
| 146 | gmx h2order -d option | Fix non-funtioning gmx h2order -d option | A fix for an option that would always take the normal along the z-axis | software | 1 |
| 147 | gmx hbond | Fix uninitialized variable warnings in gmx hbond | A fix to prevent garbage output due to uninitialized memory | software | 34 |
| 148 | gmx hbond-legacy | gmx hbond-legacy | A legacy version of the gmx hbond tool for analyzing hydrogen bonds | software | 11 |
| 149 | gmx helix | gmx helix | A GROMACS tool to compute properties of helical structures | software | 7 |
| 150 | gmx helixorient | gmx helixorient | A GROMACS tool to calculate the orientation of an alpha helix | software | 6 |
| 151 | gmx hydorder | gmx hydorder | A GROMACS tool to compute tetrahedrality order parameters | software | 7 |
| 152 | gmx insert-molecules | gmx insert-molecules | A GROMACS tool to insert molecules into a system, e.g., for solvation | software | 19 |
| 153 | gmx lie | Fix incorrect reading of certain older tpr files | A fix for incorrect reading of some older tpr files, which could lead to memory allocation errors | software | 8 |
| 154 | gmx make_edi | gmx make_edi | A GROMACS tool to generate an input file for essential dynamics sampling | software | 10 |
| 155 | gmx make_ndx | gmx make_ndx | A GROMACS tool to create special index groups for analysis | software | 17 |
| 156 | gmx make_ndx chain IDs | Made gmx make_ndx keep chain IDs | A fix to prevent old style structure file reading from overwriting chain IDs | software | 0 |
| 157 | gmx mdmat | gmx mdmat | A GROMACS tool to create distance matrices between residue pairs | software | 9 |
| 158 | gmx mdrun -gcom | gmx mdrun -gcom | A feature for less frequent communication between PP ranks, which was removed | software | 2 |
| 159 | gmx mindist | gmx mindist | A GROMACS tool to compute the minimum distance between groups of atoms | software | 14 |
| 160 | gmx mk_angndx | gmx mk_angndx | A GROMACS tool to create an index file for angle/dihedral analysis | software | 9 |
| 161 | gmx morph | gmx morph | A tool for interpolating between conformations, which was removed | software | 2 |
| 162 | gmx nmr | gmx nmr | A GROMACS tool to extract distance or orientation restraint data from an energy file | software | 10 |
| 163 | gmx nmtraj | gmx nmtraj | A GROMACS tool to generate a virtual trajectory from a normal mode eigenvector | software | 8 |
| 164 | gmx nonbonded-benchmark | gmx nonbonded-benchmark | A GROMACS tool for benchmarking the performance of non-bonded kernels | software | 6 |

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| 165 | gmx order | gmx order | A GROMACS tool to compute order parameters, typically for lipid tails | software | 15 |
| 166 | gmx pairdist | gmx pairdist | A GROMACS tool to calculate pairwise distances between selections | software | 12 |
| 167 | gmx polystat | gmx polystat | A GROMACS tool to plot static properties of polymers | software | 7 |
| 168 | gmx potential | gmx potential | A GROMACS tool to compute the electrostatic potential across the box | software | 12 |
| 169 | gmx principal | gmx principal | A GROMACS tool to calculate the three principal axes of inertia | software | 7 |
| 170 | gmx rama | gmx rama | A GROMACS tool to compute and plot Ramachandran (phi/psi) angles | software | 9 |
| 171 | gmx report-methods | gmx report-methods | A GROMACS tool to report basic system information from a run input file | software | 6 |
| 172 | gmx rms -nomw | gmx rms -nomw | An option to disable mass-weighting, which now correctly avoids guessing atom masses | identifier | 0 |
| 173 | gmx rmsdist | gmx rmsdist | A GROMACS tool to compute the RMS deviation of atom distances | software | 9 |
| 174 | gmx rotacf | gmx rotacf | A GROMACS tool to calculate the rotational correlation function | software | 8 |
| 175 | gmx rotmat | gmx rotmat | A GROMACS tool to plot the rotation matrix for least-squares fitting | software | 6 |
| 176 | gmx saltbr | gmx saltbr | A GROMACS tool to analyze the distance between charged groups (salt bridges) | software | 6 |
| 177 | gmx sans-legacy | gmx sans-legacy | A legacy GROMACS tool to compute Small-Angle Neutron Scattering (SANS) spectra | software | 9 |
| 178 | gmx sasa | gmx sasa | A GROMACS tool to compute solvent accessible surface area | software | 9 |
| 179 | gmx saxs-legacy | gmx saxs-legacy | A legacy GROMACS tool to calculate Small-Angle X-ray Scattering (SAXS) structure factors | software | 9 |
| 180 | gmx scattering | gmx scattering | A modern analysis tool that replaces the older gmx sans and gmx saxs tools | software | 8 |
| 181 | gmx sham | gmx sham | A GROMACS tool for making multi-dimensional free-energy, enthalpy, and entropy plots | software | 8 |
| 182 | gmx sigeps | gmx sigeps | A GROMACS tool to convert between different Lennard-Jones parameter representations | software | 6 |
| 183 | solvate | gmx solvate | Solvates a molecule within a pre-equilibrated solvent box | software | 58 |
| 184 | gmx sorient | gmx sorient | A GROMACS tool to analyze solvent orientation around solutes | software | 7 |
| 185 | gmx spatial | gmx spatial | An analysis tool for spatial distribution functions, with several bug fixes | software | 11 |
| 186 | gmx spol | gmx spol | A GROMACS tool to analyze dipoles around a solute, useful for polarizable water | software | 7 |
| 187 | gmx tcaf | gmx tcaf | A GROMACS tool to compute transverse current autocorrelations for viscosity estimation | software | 9 |
| 188 | gmx tool -tu | Time output unit fixes | A fix to produce the correct time unit string in xvg files for microseconds or larger | software | 1 |
| 189 | gmx traj | gmx traj | A GROMACS tool to plot coordinates, velocities, forces, and box vectors from a trajectory | software | 19 |
| 190 | trjcat | gmx trjcat | A GROMACS tool for concatenating trajectory files | software | 18 |
| 191 | gmx trjcat -demux | Fix default output with gmx trjcat -demux | A fix to ensure files are written when using the default file name output | software | 2 |
| 192 | gmx trjorder | gmx trjorder | A GROMACS tool to order molecules according to their distance to a reference group | software | 7 |
| 193 | gmx tune_pme | gmx tune_pme | A GROMACS tool to systematically benchmark and optimize PME settings | software | 25 |
| 194 | gmx velacc | gmx velacc | A GROMACS tool to compute the velocity autocorrelation function | software | 9 |
| 195 | gmx view | gmx view | A built-in viewer that has been removed from GROMACS | software | 2 |
| 196 | gmx wham with angle geometries | Fix gmx wham with angle geometries | A fix for incorrect unit conversion in gmx wham | software | 1 |
| 197 | gmx wheel | gmx wheel | A GROMACS tool to plot a helical wheel representation of a sequence | software | 7 |
| 198 | gmx xpm2ps | gmx xpm2ps | A tool for which numerous minor bugs introduced since GROMACS 5.1 were fixed | software | 19 |
| 199 | gmx-msd | gmx-msd | A GROMACS tool to compute the mean square displacement (MSD) of atoms from a set of initial positions | software | 1 |

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| 200 | gmx-nmeig | gmx-nmeig | A GROMACS tool to calculate the eigenvectors/values of a (Hessian) matrix | software | 1 |
| 201 | gmx-nmens | gmx-nmens | A GROMACS tool to generate an ensemble around an average structure in a subspace that is defined by a set of normal modes (eigenvectors) | software | 1 |
| 202 | gmx-pme_error | gmx-pme_error | A GROMACS tool to estimate the error of the electrostatic forces if using the sPME algorithm | software | 1 |
| 203 | gmx-rdf | gmx-rdf | A GROMACS tool to calculate radial distribution functions from one reference set of position to one or more sets of positions | software | 3 |
| 204 | gmx-rms | gmx-rms | A GROMACS tool to compare two structures by computing the root mean square deviation (RMSD), the size-independent rho similarity parameter (rho) or the scaled rho (rhosc) | software | 1 |
| 205 | gmx-rmsf | gmx-rmsf | A GROMACS tool to compute the root mean square fluctuation (RMSF, i.e. standard deviation) of atomic positions in the trajectory after (optionally) fitting to a reference frame | software | 1 |
| 206 | gmx-select | gmx-select | A GROMACS tool to write out basic data about dynamic selections | software | 1 |
| 207 | gmx-trajectory | gmx-trajectory | A GROMACS tool to print coordinates, velocities, and/or forces for selections | software | 1 |
| 208 | gmx-wham | gmx-wham | A GROMACS tool to perform weighted histogram analysis after umbrella sampling | software | 1 |
| 209 | GMX_ASSERT | GMX_ASSERT | A GROMACS macro for assertions in debug and development builds | software | 4 |
| 210 | GMX_CUDA_GRAPH | GMX_CUDA_GRAPH | An environment variable to activate the experimental CUDA Graphs feature | identifier | 3 |
| 211 | GMX_DSSP_PROGRAM_PATH | GMX_DSSP_PROGRAM_PATH | A new way to configure the default path for the dssp executable | identifier | 1 |
| 212 | GMX_GPU_NB_CLUSTER_SIZE | GMX_GPU_NB_CLUSTER_SIZE | The current CMake variable for setting the GPU non-bonded cluster size | identifier | 4 |
| 213 | GMX_GPU_PME_DECOMPOSITION | GMX_GPU_PME_DECOMPOSITION | An environment variable to enable the experimental GPU-based PME decomposition feature | identifier | 2 |
| 214 | GMX_INSTALL_NBLIB_API | GMX_INSTALL_NBLIB_API | A CMake option to install the NB-Lib API, now initialized from BUILD_SHARED_LIBS | identifier | 5 |
| 215 | gmx_mpi | gmx_mpi | The executable name for an MPI-enabled GROMACS build | software | 27 |
| 216 | GMX_OPENCL_NB_CLUSTER_SIZE | GMX_OPENCL_NB_CLUSTER_SIZE | A deprecated CMake variable for setting the OpenCL non-bonded cluster size | identifier | 4 |
| 217 | GMX_RELEASE_ASSERT | GMX_RELEASE_ASSERT | A GROMACS macro for assertions that are active in all build types | software | 3 |
| 218 | GMX_THROW | GMX_THROW | A GROMACS macro for throwing exceptions | software | 0 |
| 219 | GMX_VERSION_STRING_OF_FORK | GMX_VERSION_STRING_OF_FORK | A CMake variable to identify forked versions of GROMACS | identifier | 3 |
| 220 | gmxapi | gmxapi | A Python package for scripting GROMACS simulations and analysis | software | 468 |
| 221 | gmxapi-cppdocs target | gmxapi-cppdocs | A build target for generating the gmxapi C++ API documentation | software | 0 |
| 222 | gmxapi.commandline_operation | gmxapi.commandline_operation | A gmxapi function to wrap command-line tools, with updated directory handling | software | 9 |
| 223 | gmxapi.commandline_operation runtime arguments | gmxapi.mdrun accepts arbitrary runtime arguments | A feature to pass arbitrary command-line arguments to command-line operations via gmxapi | software | 0 |
| 224 | gmxapi.mdrun stdout/stderr | gmxapi.mdrun now captures STDOUT and STDERR | New output attributes from gmxapi.mdrun that capture the standard output and error streams of the simulation | software | 0 |
| 225 | gmxapi.mdrun().output.directory | gmxapi.mdrun().output.directory | A new output attribute from gmxapi.mdrun that provides the path to the simulation working directory | software | 1 |
| 226 | modify_input | gmxapi.modify_input | A gmxapi function to modify simulation input parameters | software | 5 |
| 227 | read_tpr | gmxapi.read_tpr | A gmxapi function to create simulation input from a TPR file | software | 8 |
| 228 | GMXLIB | GMXLIB | An environment variable to provide alternative locations for GROMACS data files | identifier | 17 |

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| 229 | gmxpre-config.h | gmxpre-config.h | A generated header file included first, containing pre-configuration defines | data format | 2 |
| 230 | GMXRC | GMXRC | A script that sets up the necessary environment variables for running GROMACS | software | 29 |
| 231 | GPU API considerations | GPU API considerations | Specific coding guidelines for writing code that targets GPUs (CUDA, OpenCL, SYCL) | process | 2 |
| 232 | GPU direct communication | GPU direct communication | A technology allowing GPUs to communicate directly without involving the CPU | method\|software | 6 |
| 233 | GPU version of LINCS | Bug fix for the GPU version of LINCS in multiple domain case | A fix for a memory re-allocation issue in the GPU LINCS implementation | software | 1 |
| 234 | graph and modular simulations | Fix simulations using graph and modular simulations | A fix for a segmentation fault when using the modular simulator and a graph object | software | 1 |
| 235 | GROMOS | GROMOS | A set of united-atom force fields and a simulation package | model\|software | 78 |
| 236 | GROMOS force fields warning | Added warning with the use of GROMOS force fields | A new warning in grompp regarding the use of GROMOS force fields with single-range cut-offs | software | 0 |
| 237 | grompp | gmx grompp | The GROMACS preprocessor that creates a run input file | software | 245 |
| 238 | grompp with frozen system | Fix crash of grompp when the whole system is frozen | A fix for a segmentation fault when the entire system was frozen | software | 0 |
| 239 | Hydrogen database | hdb | A database that provides rules for adding hydrogen atoms | data source\|data format | 11 |
| 240 | HeFFTe | HeFFTe | A library for scalable Fast Fourier Transforms on distributed systems | software | 30 |
| 241 | Helical wheel | helical wheel | A 2D projection of a helix used to visualize the distribution of residue types | model | 3 |
| 242 | Helix radius | Helix radius | The RMS deviation of C-alpha atoms from the helical axis | measure | 1 |
| 243 | Helix rise | Rise per residue | The translation along the helical axis per residue | measure | 0 |
| 244 | Helix twist | Twist | The average helical angle per residue | measure | 0 |
| 245 | Hessian matrix | Hessian matrix | A square matrix of second-order partial derivatives of a function | model | 13 |
| 246 | HPC Container Maker | HPC Container Maker | A tool from NVIDIA for generating container specification files | software | 2 |
| 247 | Hungarian notation | hungarian notation | A naming convention where a prefix indicates the variable's type (e.g., 'b' for boolean) | identifier | 2 |
| 248 | hwloc | hwloc | A hardware locality library for which support for older versions is being removed | software | 28 |
| 249 | hwloc version 1 | Support for version 1 of the hardware locality library hwloc | Support for this older version of hwloc is being removed | software | 0 |
| 250 | IBM VMX SIMD | IBM VMX SIMD | A SIMD instruction set for PowerPC, a deprecated platform | software | 1 |
| 251 | IBM_VSX support | Give clearer message about not detecting IBM_VSX support in gcc > 9 | A fix to provide a more informative error message from CMake | software | 1 |
| 252 | ICC NextGen | Add support for ICC NextGen | Support for the Intel Compiler based on LLVM technology | software | 1 |
| 253 | ImageMagick | ImageMagick | A software suite for image manipulation, used as a dependency for documentation | software | 2 |
| 254 | Index editor | index editor | An interactive tool within gmx make_ndx for creating and manipulating index groups | software | 1 |
| 255 | Index File | .ndx | Specifies custom groups of atoms for analysis or simulation | data format | 143 |
| 256 | ingroup | \ingroup | A Doxygen command to add an item to an existing documentation group | software | 11 |
| 257 | initial DLB state | Fixed initial DLB state reporting | A fix for incorrect reporting of the initial dynamic load balancing state in the log file | software | 2 |
| 258 | inlibraryapi | \inlibraryapi | A GROMACS-specific Doxygen command to mark a header as part of the library API | software | 5 |
| 259 | inpublicapi | \inpublicapi | A GROMACS-specific Doxygen command to mark a header as part of the public API | software | 7 |
| 260 | install-guide target | install-guide | A build target that generates the plain-text INSTALL file | software | 0 |

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| 261 | integer overflow with dispersion correction | Avoid integer overflow when using dispersion correction | A fix for an integer overflow in the index type for dispersion correction | software | 0 |
| 262 | Intel clang-based compiler | icx/icpx | The newer Intel compiler based on Clang, which is now supported | software | 1 |
| 263 | Intel classic compiler | icc/icpc | The classic Intel C/C++ compiler, which is no longer supported | software | 2 |
| 264 | Intel integrated GPUs | Intel integrated GPUs are now supported for GPU offload with OpenCL | A feature to offload nonbonded tasks to integrated Intel GPUs | software | 6 |
| 265 | Interactive molecular dynamics (IMD) | Interactive molecular dynamics (IMD) | A technique that allows real-time interaction with a running simulation | method | 2 |
| 266 | internal | \internal | A Doxygen command to mark documentation for inclusion only in the full documentation | software | 91 |
| 267 | issues | issues | The feature in gitlab used for tracking bugs and feature requests | process | 219 |
| 268 | Job parameters | Job parameters | Keywords in the .gitlab-ci.yml file that control how a job is executed | identifier | 3 |
| 269 | kJ/mol | kJ mol-1 | Kilojoules per mole, a unit of energy | unit | 21 |
| 270 | kJ/mol/nm^2 | kJ/mol/nm^2 | A unit for solvation free energy per area | unit | 2 |
| 271 | L-BGFS minimizer | L-BGFS minimizer | A minimization algorithm that could fail on a number of systems, which was fixed | algorithm | 1 |
| 272 | Labels | Labels | A feature in gitlab to categorize and filter issues and merge requests | identifier | 17 |
| 273 | LD_LIBRARY_PATH | LD_LIBRARY_PATH | An environment variable that lists directories to search for shared libraries | identifier | 3 |
| 274 | Legacy API | Legacy API | A statement that all headers in the src directory are for internal consumption and subject to change | software | 7 |
| 275 | Legendre polynomial | Legendre polynomial | A class of orthogonal polynomials used in vector correlation functions | model | 15 |
| 276 | libgromacs CMake target | Fix INTERFACE_INCLUDE_DIRECTORIES for libgromacs CMake target | A fix for a malformed CMake target referencing non-existent directories | software | 5 |
| 277 | libinternal | \libinternal | A GROMACS-specific Doxygen command to mark documentation for exclusion from the public API | software | 22 |
| 278 | Libtorch | Libtorch | The C++ distribution of the PyTorch machine learning framework | software | 13 |
| 279 | LINCS | LINCS | A linear constraint solver algorithm | algorithm | 80 |
| 280 | Linear angle potential | linear angle | A special potential for angles that are supposed to be linear (180 degrees) | model | 6 |
| 281 | linkchecker | linkchecker | A tool used to check for broken links in the documentation | software | 2 |
| 282 | LJ PME free energy | Fixed free energy calculations with LJ PME | A fix for wrong long-range corrections with vdwtype=pme in free energy calculations | method | 0 |
| 283 | LJ repulsion force switching on GPUs | Fix incorrect LJ repulsion force switching on GPUs | A fix for an incorrect sign in the LJ repulsion force switching coefficient on GPUs | software | 2 |
| 284 | LJ-PME and dispersion correction | Fix assertion failure with LJ-PME and dispersion correction | A fix for an assertion failure during PME tuning with this combination | software | 1 |
| 285 | Luzar and Chandler model | model of Luzar and Chandler | A model for analyzing the kinetics of hydrogen bond breaking and formation | model | 0 |
| 286 | make-release-build.py | make-release-build.py | A script for automating release-related build and pipeline tasks | software | 2 |
| 287 | man target | man | A build target that generates man pages for GROMACS programs | software | 2 |
| 288 | manual target | manual | A build target that generates the reference manual in PDF format | software | 1 |
| 289 | Velocity Verlet integrator | md-vv | A numerical integrator that is more accurate than leap-frog | algorithm | 6 |

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| 290 | mdrun | gmxapi.mdrun | A gmxapi function to create an MD simulation operation | software | 693 |
| 291 | mdrun -ddorder pp_pme | mdrun -ddorder pp_pme | A fix for a deadlock that occurred during initialization with this rank ordering | software | 1 |
| 292 | mdrun -deffnm | mdrun -deffnm | A deprecated mdrun option for setting a default file name prefix | identifier | 12 |
| 293 | mdrun -multidir | Fix fatal error with mdrun -multidir with more than 1 rank per simulation | A fix for a fatal error with this option | software | 10 |
| 294 | mdrun -multidir with shared state | Add fatal error for mdrun -multidir when simulations sharing state start at different step | A fix to issue a fatal error when simulations in a multi-simulation run start at different steps | software | 0 |
| 295 | mdrun -nsteps option | Fixed mdrun -nsteps option | A fix for the deprecated -nsteps option to allow extension of simulations | identifier | 1 |
| 296 | mdrun -update auto | mdrun -update auto | An option that now defaults to GPU update if supported, giving a significant performance improvement | identifier | 2 |
| 297 | mdrun MPI rank count | Allow large prime factors in the mdrun MPI rank count | A fix to allow domain decomposition to run with large prime factors in the MPI rank count | software | 1 |
| 298 | mdrun with multiple ranks and separate PME ranks | Fix deadlock in mdrun runs with multiple ranks and separate PME ranks | A fix for a deadlock that could occur before PP-PME balancing | software | 0 |
| 299 | mdrun with shells and GPU update | Avoid mdrun assertion failure when running with shells and update on a GPU | A fix to make mdrun fall back to CPU or error out when attempting this unsupported combination | software | 0 |
| 300 | mdrun-only build | The mdrun-only build of GROMACS | A removed build configuration that was no longer easier to build or test | software | 7 |
| 301 | Mean Square Displacement | MSD | A measure of the average distance a particle travels over time | measure | 10 |
| 302 | merge requests | merge requests | The feature in gitlab used for submitting and reviewing code changes | process | 8 |
| 303 | MiMiC | MiMiC | A multiscale modeling environment for QM/MM simulations | software | 41 |
| 304 | Minimum image convention | minimum image convention | A convention in periodic systems where interactions are calculated with the closest periodic image | model\|method | 7 |
| 305 | missing DD interactions | Avoid deadlock when checking for missing DD interactions | A fix for a deadlock that occurred when missing bonded interactions were detected after domain decomposition | software | 1 |
| 306 | modified source files in release tarballs | Fix check for modified source files in release tarballs | A fix to ensure modifications to the source tree are picked up after the build directory is generated | software | 1 |
| 307 | Molecular order tensor | molecular order tensor | A tensor describing the orientational order of molecules | measure | 2 |
| 308 | molecule indexing | Fixes the unexpected change in molecule indexing in output after simulation | A fix to ensure repeat molecules are numbered consecutively | software | 2 |
| 309 | Moments of inertia | moments of inertia | A measure of an object's resistance to rotational motion | measure | 2 |
| 310 | Morse potential | Morse | A potential function describing bond stretching, allowing for dissociation | model | 6 |
| 311 | MSD tensor | MSD tensor | A tensor describing the mean square displacement in x, y, and z directions | measure | 1 |
| 312 | MSVC build | Fix building with MSVC | A fix for a missing header that caused build failure with MSVC | software | 0 |
| 313 | MSVC SIMD flags | Update MSVC SIMD flags | Newly supported SIMD flags that may improve performance on Windows | software | 1 |
| 314 | Multiple Time-Stepping | mts | An integration scheme using different timesteps for different forces | algorithm\|method | 9 |

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| 315 | N-body virtual sites with DD | Fix index handling of N-body virtual sites with domain decomposition | A fix for incorrect indexing of N-body virtual sites in the domain decomposition code | software | 0 |
| 316 | Naming conventions | Naming conventions | Guidelines for naming files, variables, functions, and classes | process | 3 |
| 317 | Nbnxm kernels | Nbnxm non-bonded pair kernels | Highly optimized kernels for non-bonded force calculations in GROMACS | software\|algorithm | 3 |
| 318 | nm | nm | Nanometer, a unit of length | unit | 236 |
| 319 | nmeig | nmeig does thermochemistry | A tool that now generates thermochemical properties from a Hessian matrix | software | 19 |
| 320 | NMR averaged distances | NMR averaged distances | Distances averaged according to 1/r^3 or 1/r^6, relevant for NMR NOE data | measure | 1 |
| 321 | NMR restraints with modular simulator | Fix NMR restraints using modular simulator | A fix for NMR restraints not working as expected under the modular simulator | software | 0 |
| 322 | non-dynamical integrator | Updated message on using GPU with non-dynamical integrator | A clearer message explaining why GPU PME/bonded forces are not supported with non-dynamical integrators | software | 2 |
| 323 | Nose-Hoover coupling | Nose-Hoover coupling | A method for temperature control that generates a canonical ensemble | method\|algorithm | 0 |
| 324 | Nosé-Hoover thermostat | Nosé-Hoover thermostat | A deterministic thermostat for controlling temperature in molecular dynamics | algorithm\|method | 5 |
| 325 | nstcalcenergy | nstcalcenergy | An mdp option for the frequency of energy calculations | identifier | 24 |
| 326 | nstcomm | nstcomm | The frequency for center-of-mass motion removal, no longer modified by grompp | identifier | 6 |
| 327 | NVIDIA Turing GPUs | Added code generation support for NVIDIA Turing GPUs | A feature to directly target the Turing architecture with the nvcc compiler | software | 4 |
| 328 | Occupancy fraction | occupancy fraction | The fraction of frames in which a position is selected | measure | 2 |
| 329 | oneAPI | oneAPI | An open, cross-industry standard for unified programming across different architectures | software | 61 |
| 330 | OpenCL | OpenCL | An open standard for parallel programming of heterogeneous systems | software\|method | 165 |
| 331 | OpenCL on Volta and Turing | Document known issues with OpenCL on Volta and Turing | Documentation of known issues with OpenCL on these NVIDIA GPU architectures | data source | 1 |
| 332 | OPLS | OPLS | Optimized Potentials for Liquid Simulations force field family | model | 36 |
| 333 | orientation restraints | Avoid overzealous program abort with orientation restraints | A fix to prevent mdrun from aborting on checking orientation restraints in multiple molecules when none were applied | software | 28 |
| 334 | OSX build | Fix building on OSX | A fix for a missing include that prevented compilation on macOS | software | 0 |
| 335 | P-LINCS | P-LINCS | A parallel version of the LINCS constraint algorithm | algorithm | 12 |
| 336 | P3M-AD | P3M-AD | Particle-Particle Particle-Mesh algorithm with analytical derivative | algorithm\|method | 9 |
| 337 | package_source target | package_source | A CPack target that builds a source package for release | software | 0 |
| 338 | pairlist buffer on Intel GPUs | Fix too small pairlist buffer on Intel GPUs | A fix for a too-small pairlist buffer on Intel GPUs, which assumed a 4x4 instead of 4x2 atom-cluster pair kernel | software | 1 |
| 339 | Parrinello-Rahman and md-vv checkpoints | Fix checkpoint restarts using Parrinello-Rahman and md-vv | A fix to allow reading checkpoints created with these methods in the modular simulator | software | 1 |
| 340 | Parrinello-Rahman coupling | Parrinello-Rahman coupling | A method for pressure control that allows for box shape changes | method\|algorithm | 8 |
| 341 | pdb2gmx | gmx pdb2gmx | Generates a GROMACS topology from a PDB structure file | software | 136 |
| 342 | Persistence length | persistence length | A measure of the stiffness of a polymer chain | measure | 3 |
| 343 | PLUMED | PLUMED | A library for free energy calculations and analysis that can be coupled with GROMACS | software\|method | 34 |
| 344 | Particle-mesh Ewald | PME | A fast Fourier-based method for long-range electrostatics | algorithm\|method | 10 |
| 345 | PME decomposition | PME decomposition | A feature to offload PME calculations to multiple GPUs, now with support for CUDA and SYCL backends | method\|algorithm | 15 |

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| 346 | PME forces with FE | Actually fix PME forces with FE without perturbed q/LJ | A fix for incorrectly ignoring PME mesh forces on non-perturbed atoms in certain FE scenarios | software | 2 |
| 347 | PME long-ranged interaction GPU offload | PME long-ranged interaction GPU offload now available with OpenCL | A feature to offload PME calculations to the GPU using OpenCL on all supported vendors | method\|software | 1 |
| 348 | PME Mixed mode | PME Mixed mode | A PME execution mode that was disabled for FEP simulations due to incorrectness | method | 2 |
| 349 | PME on GPU with charge-free FEP | PME on GPU when running free energy perturbations not involving charges | A new feature allowing PME to run on the GPU for certain free energy calculations | method | 0 |
| 350 | PME OpenCL on Apple | Disable PME OpenCL on Apple | A fix to disable OpenCL PME on Apple platforms due to compiler failures | software | 1 |
| 351 | Polarizable water | polarizable water | Water models that can respond to an electric field by changing their dipole moment | model | 1 |
| 352 | Position restraints | position_restraints | Harmonic potentials used to keep atoms close to reference positions | model | 49 |
| 353 | Potential of Mean Force | Potential of Mean Force | The potential energy as a function of a reaction coordinate | measure\|model | 11 |
| 354 | PQR formatting | Fix PQR formatting | A fix for incorrect formatting in tools that use PQR files | data format | 1 |
| 355 | FFTW with clang and AVX-512 SIMD | Prevented internal build of FFTW with clang and AVX-512 SIMD | A fix to prevent the internal FFTW build from attempting an unsupported compilation | software | 1 |
| 356 | Principal axes of inertia | principal axes of inertia | The three mutually orthogonal axes about which the moment of inertia is maximized | measure | 6 |
| 357 | Principal Components | principal components | Projections of a trajectory onto the eigenvectors of its covariance matrix | measure | 10 |
| 358 | Progressive fit | progressive | A trajectory fitting method where each frame is fitted to the previously fitted frame | method | 1 |
| 359 | COM pulling | pull | Applying a force to the center of mass of a group of atoms | method | 5 |
| 360 | Pull code | pull code | A GROMACS module for applying forces or constraints to collective variables | software\|method | 24 |
| 361 | pull group index handling | Fix pull group index handling | A fix for incorrect validation of pull group indices in grompp | software | 1 |
| 362 | pull-fout-average | pull-fout-average | A new option to enable output of average pull forces | identifier | 2 |
| 363 | pull-pbc-ref-from-prev-step-com | pull-pbc-ref-from-prev-step-com | An added option to use the COM of the previous step as a PBC reference in pulling | identifier | 1 |
| 364 | pull-xout-average | pull-xout-average | A new option to enable output of average pull positions | identifier | 2 |
| 365 | pullx.xvg | pullx.xvg | A pull code output file that is now correctly written during a rerun | data format | 11 |
| 366 | pybind11 dependency | pybind11 dependency | The pybind11 library is no longer bundled and must be provided externally | software | 1 |
| 367 | Quantum corrections | quantum corrections | Corrections to classical simulations to account for quantum effects, e.g., on heat capacity | method | 3 |
| 368 | Quartic angle potential | quartic angle | An angle potential defined by a quartic function of the angle | model | 1 |
| 369 | Residue to building block map file | r2b | File for mapping residue names to force-field building block names | data format | 0 |
| 370 | Radial distribution function (RDF) | radial distribution functions | A function that describes how density varies as a function of distance from a reference particle | measure | 2 |
| 371 | Radius of gyration | radius of gyration | A measure of the size of a molecule or group of atoms | measure | 17 |
| 372 | RAII | RAII | Resource Acquisition Is Initialization, a C++ programming technique for resource management | method | 1 |
| 373 | Ramachandran plot | Ramachandran plot | A plot of the phi and psi backbone dihedral angles of amino acids | method | 4 |
| 374 | RDCYCLE | RDCYCLE | A deprecated instruction on RISC-V for reading the cycle counter | software | 2 |
| 375 | RDRAND on Ryzen | Added workaround for RDRAND not always returning random numbers on Ryzen | A workaround for a hardware bug in the random number generator on some AMD CPUs | software | 0 |

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| 376 | RDTIME | RDTIME | An instruction on RISC-V that replaces the deprecated RDCYCLE for security reasons | software | 2 |
| 377 | RDTSCP on x86 | Only check for RDTSCP on x86 platforms | A change to only check for this instruction on relevant platforms | software | 1 |
| 378 | Real space | real space | The direct, coordinate-space representation of the simulation box | model | 4 |
| 379 | Reciprocal space | reciprocal space | The Fourier-space representation of the simulation box, used in Ewald methods | model | 18 |
| 380 | Relocatable binaries | Relocatable binaries | The ability for installed GROMACS binaries to be moved to a different location and still function | software | 8 |
| 381 | Replica exchange | replica exchange | An enhanced sampling method that exchanges configurations between temperatures or Hamiltonians | method\|algorithm | 32 |
| 382 | report-methods | Implement writing of LaTeX methods in report-methods | A new tool to generate a summary of simulation methods | software | 9 |
| 383 | ResourceManager | ResourceManager | A gmxapi component for managing resources in MPI ensembles, with improved awareness | software | 2 |
| 384 | Restraint module for gmxapi | Restraint module for gmxapi MD extension code | New functionality for registering externally compiled MD extensions at runtime | software | 1 |
| 385 | Restraint lambdas | restraint-lambdas | The free energy coupling parameter for restraint interactions | measure | 0 |
| 386 | Restricted bending potential | Restricted bending potential | A potential that prevents bond angles from reaching 180 degrees | model | 11 |
| 387 | rho similarity parameter | rho similarity parameter | A size-independent measure of structural similarity | measure | 1 |
| 388 | ROCm | ROCm | AMD's open-source software platform for GPU computing | software | 34 |
| 389 | Root Mean Square Deviation (RMSD) | root mean square deviation (RMSD) | A measure of the average distance between the atoms of superimposed structures | measure | 2 |
| 390 | Root Mean Square Fluctuation (RMSF) | root mean square fluctuation (RMSF) | A measure of the deviation of an atom's position from its average position | measure | 0 |
| 391 | Rotation matrix | ?(t) | A time-dependent matrix that describes the orientation of the reference structure | model | 11 |
| 392 | Rotational correlation function | rotational correlation function | A function that describes the time correlation of a molecule's orientation | measure | 6 |
| 393 | Rotational kinetic energy | translational and rotational kinetic energy | The kinetic energy associated with the rotational motion of a group | measure | 3 |
| 394 | RPATH | RPATH | A path embedded in an executable that specifies where to find shared libraries | identifier | 11 |
| 395 | Salt bridge | salt bridges | A non-covalent interaction between two oppositely charged residues | chemical entity | 1 |
| 396 | SANS intensity | SANS intensity | The scattering intensity as a function of the scattering vector q for SANS | measure | 2 |
| 397 | Scattering intensity | scattering intensity | The intensity of scattered radiation as a function of the scattering angle | measure | 2 |
| 398 | Schedules and triggers | Schedules and triggers | Mechanisms for running GitLab CI pipelines automatically or on-demand | process | 1 |
| 399 | scripted_gmx_docker_builds.py | scripted_gmx_docker_builds.py | A script for generating Dockerfiles for GROMACS CI testing images | software | 7 |
| 400 | SETTLE | SETTLE | An analytical algorithm for constraining the geometry of water molecules | algorithm | 29 |
| 401 | SHAKE | SHAKE | A popular algorithm for satisfying bond constraints | algorithm | 44 |
| 402 | Shear viscosity | shear viscosity | A measure of a fluid's resistance to shear stress | measure | 8 |
| 403 | Sigma and epsilon | sigma and epsilon | Parameters for the Lennard-Jones potential representing atomic size and interaction strength | model | 2 |
| 404 | Simple Point Charge (SPC) water | Simple Point Charge water (SPC) | A commonly used 3-site rigid water model | model | 0 |
| 405 | Single histogram analysis method | single histogram analysis method | A reweighting method to calculate properties at different state points from a single simulation | method | 1 |

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| 406 | skewed box with modular simulator | Correct skewed box using modular simulator without DD | A fix to check for overly skewed boxes when using the modular simulator without domain decomposition | software | 0 |
| 407 | Solvation free energy | solvation free energies | The free energy change associated with transferring a molecule from vacuum to solvent | measure | 3 |
| 408 | Solvent Accessible Surface Area (SASA) | solvent accessible surface areas | The surface area of a biomolecule that is accessible to a solvent | measure | 0 |
| 409 | Source tree checker scripts | Source tree checker scripts | A set of Python scripts for checking source code consistency and documentation | software | 8 |
| 410 | Spatial Distribution Function (SDF) | spatial distribution function | A function that describes the 3D density distribution of a group of atoms | measure | 0 |
| 411 | Special targets | Special targets | CMake targets for performing specific developer or CI tasks | software | 3 |
| 412 | splitat | splitat | An option in gmx make_ndx for which an invalid memory access was fixed | identifier | 1 |
| 413 | splitres | splitres | An option in gmx make_ndx for which the old behavior of printing all atoms has been restored | identifier | 3 |
| 414 | Splitting parameter | splitting parameter | A parameter (ewald_beta) that divides the Ewald sum into real and reciprocal space parts | model | 2 |
| 415 | ssh key | ssh key | A cryptographic key pair used for secure authentication with gitlab | identifier | 2 |
| 416 | Standard Entropy | Standard Entropy | The entropy content of one mole of substance under standard state conditions | measure | 2 |
| 417 | static_assert | static_assert | A C++ feature to perform assertions at compile time | software | 2 |
| 418 | Stochastic cell rescaling barostat | Stochastic cell rescaling barostat | A first-order stochastic barostat that has been implemented for equilibration and production | method\|algorithm | 3 |
| 419 | Stochastic Dynamics | Stochastic Dynamics | A simulation method that includes random forces to mimic solvent effects | method | 11 |
| 420 | Stochastic Dynamics integrator | SD integrator | An integrator that includes stochastic forces to represent a heat bath | algorithm\|integrator | 2 |
| 421 | Style guidelines | Style guidelines | Rules and conventions for code formatting and naming in GROMACS | process | 16 |
| 422 | Subgraph | gmxapi.operation.Subgraph | A gmxapi construct to group operations for repeated execution or modularity | software | 29 |
| 423 | SYCL | SYCL | A cross-platform abstraction layer for programming heterogeneous processors | software | 90 |
| 424 | tau-p | tau-p | The time constant for pressure coupling, with a changed default value | measure | 13 |
| 425 | Termini database | tdb | A database for modifying terminal residues of a polymer | data source\|data format | 2 |
| 426 | temperature calculation with partial COM removal | Fix temperature calculation when center of mass motion is removed for part of the system | A fix for incorrectly lowered degrees of freedom in this uncommon case | software | 0 |
| 427 | Termini | ter | The N- and C-terminal ends of a polypeptide chain | chemical entity | 17 |
| 428 | Test particle insertion | Test particle insertion | A method for calculating chemical potentials, which had a bug in dispersion correction | method | 11 |
| 429 | test target | test | A CTest target that runs registered tests without building them | software | 3 |
| 430 | tests target | tests | A build target that builds all test binaries | software | 2 |
| 431 | Tetrahedrality order parameter | tetrahedrality order parameters | A measure of the local tetrahedral arrangement of atoms, e.g., around a water molecule | measure | 0 |
| 432 | LaTeX file | tex | A document processing format, can be an output type | data format | 1 |
| 433 | Thermodynamic Integration | TI | A method to compute free energy by integrating the ensemble-averaged derivative of the Hamiltonian | method\|algorithm | 3 |
| 434 | Thermostat | Thermostats | An algorithm to control the temperature of a simulation | algorithm\|model | 43 |
| 435 | tinyxml2 linking | Fix error with tinyxml2 linking | A fix for an incorrect signature for linking this external library | software | 1 |
| 436 | Topology | Topology file (.top) | Describes molecule connectivity and interaction parameters | data format\|model | 293 |

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| 437 | Transverse current autocorrelation | tranverse current autocorrelations | The autocorrelation function of the transverse component of the current | measure | 2 |
| 438 | trigger-post-merge.py | trigger-post-merge.py | A script for manually triggering post-merge acceptance pipelines | software | 3 |
| 439 | trilinic DD code | Fix type bug in trilinic DD code | A bug fix for an issue with off-diagonal elements in domain decomposition | software | 1 |
| 440 | trjconv | gmx trjconv | A GROMACS tool for processing and converting trajectory files | software | 64 |
| 441 | trjconv -ndec | Fix trjconv -ndec | A fix to make this option work correctly with .gro files | software | 3 |
| 442 | tune_pme | Fix tune_pme | A fix for a file reading error in the tool | software | 30 |
| 443 | undefined NB kernel types | Fix possible issue with picking undefined NB kernel types | A fix for missing definitions for specific CPU reference NB kernel types | software | 1 |
| 444 | Unit-cell representation | Unit-cell representation | The way the periodic box is represented (e.g., rectangular, triclinic) | model | 2 |
| 445 | Update groups | update groups | Groups of atoms that are moved together between domains to avoid communication | method | 22 |
| 446 | Updating regression tests | Updating regression tests | The process for updating the regression test suite in conjunction with code changes | process | 3 |
| 447 | Urey-Bradley potential | Urey-Bradley potential | A potential that includes a harmonic term on the distance between 1,3-atoms | model | 1 |
| 448 | van der Waals radii | van der Waals radii | The radius of an imaginary hard sphere representing an atom | measure | 10 |
| 449 | Velocity Verlet integrators | Velocity Verlet integrators output energy averages from correct steps | A fix for how energy averages were accumulated for this integrator type | algorithm\|integrator | 6 |
| 450 | Virial | virial | A quantity related to the forces between particles, used to calculate pressure | measure | 73 |
| 451 | VkFFT | VkFFT | A multi-backend GPU-accelerated multidimensional Fast Fourier Transform library | software | 32 |
| 452 | VkFFT support | VkFFT support | Integration of the VkFFT library to provide performance improvements for GPU FFTs, especially on AMD GPUs | software | 4 |
| 453 | VMD | VMD | A molecular visualization program that can interact with GROMACS | software | 37 |
| 454 | Virtual site database | vsd | A file specifying geometries for constructing virtual sites | data source\|data format | 4 |
| 455 | webpage target | webpage | A collection target that generates the full HTML documentation website | software | 3 |
| 456 | webpage-sphinx target | webpage-sphinx | A build target that generates the Sphinx-based parts of the HTML documentation | software | 0 |
| 457 | x86 MIC | x86 MIC | Intel Many Integrated Core Architecture, a deprecated platform | software | 2 |
| 458 | Xeon Phi | Xeon Phi | A series of accelerators from Intel for which support is being removed | software | 12 |
| 459 | XPM matrix file | xpm | An ASCII file format for storing matrix data | data format | 0 |
| 460 | XVG plot file | xvg | A data file format for plotting with the Grace/Xmgr program | data format | 0 |
| 461 | Zero-point energy | Zero-point energy | The lowest possible energy that a quantum mechanical system may have | measure | 4 |
| 462 | Zwitterionic | zwitterionic | A molecule with both positive and negative charges, but a net charge of zero | state | 1 |
| 463 | GROMACS | GROMACS | A versatile package for molecular dynamics simulations | software | ### |
| 464 | Molecular Dynamics | Molecular dynamics | A computer simulation method for analyzing physical movements | method\|process | 159 |
| 465 | Structure File | .gro, .pdb | Contains atomic coordinates, optionally velocities and box dimensions | data format | 65 |
| 466 | Run Input File | .tpr | A portable binary file containing all simulation parameters | data format | 68 |
| 467 | Trajectory File | .xtc, .trr, .tng | Stores atomic coordinates over time from a simulation | data format | 63 |
| 468 | Parameter File | .mdp | Controls the parameters for a molecular dynamics simulation | data format | 5 |
| 469 | Checkpoint File | .cpt | Saves the complete state of a simulation for restarting | data format | 47 |

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|---|---|---|---|---|---|
| 470 | Energy Minimization | Energy Minimization | A process to find a low-energy conformation of a molecule | process\|method | 64 |
| 471 | Periodic Boundary Conditions | Periodic boundary conditions | An approximation to an infinite system by replicating a unit cell | model\|method | 57 |
| 472 | CMake | CMake | The build system used to compile and install GROMACS | software | 411 |
| 473 | SIMD (Single Instruction, Multiple Data) | SIMD support | A class of parallel computers in a classification | method\|model | 0 |
| 474 | SSE2 | SSE2 | A specific SIMD instruction set for x86 processors | model\|method | 5 |
| 475 | AVX | AVX_256 | A specific SIMD instruction set for x86 processors | model\|method | 26 |
| 476 | AVX-512 | AVX_512 | A specific SIMD instruction set for x86 processors | model\|method | 10 |
| 477 | GPU Acceleration | GPU support | Using graphics processing units to speed up calculations | method | 22 |
| 478 | CUDA | CUDA | NVIDIA's parallel computing platform and programming model | software\|method | 218 |
| 479 | HIP | HIP | AMD's C++ Runtime API and Kernel Language for heterogeneous computing | software\|method | 23 |
| 480 | MPI (Message Passing Interface) | MPI support | A standardized means of exchanging messages between multiple computers | software\|method | 1 |
| 481 | FFT (Fast Fourier Transform) | Fast Fourier Transform library | An algorithm to compute the discrete Fourier transform efficiently | algorithm\|software | 0 |
| 482 | Intel MKL | mkl | Intel's Math Kernel Library with optimized math routines | software | 2 |
| 483 | QM/MM (Quantum Mechanics/Molecular Mechanics) | QM/MM support | A hybrid method combining quantum and classical mechanics | method\|model | 0 |
| 484 | Colvars | Colvars | A software module for collective variable-based calculations | software | 80 |
| 485 | Non-bonded interactions | Non-bonded interactions | Interactions between atoms not linked by covalent bonds | model | 57 |
| 486 | Bonded interactions | Bonded interactions | Interactions between atoms connected by covalent bonds | model | 143 |
| 487 | NVT Ensemble | NVT | A statistical ensemble with constant number, volume, and temperature | model\|state | 0 |
| 488 | NPT Ensemble | NPT | A statistical ensemble with constant number, pressure, and temperature | model\|state | 5 |
| 489 | Reproducibility | Reproducibility | The ability to obtain bit-identical results from a simulation | state\|measure | 12 |
| 490 | Parameterization | Parameterization | The process of developing force field parameters for a molecule | process\|method | 12 |
| 491 | Double Precision | Double precision | A floating-point number format occupying 8 bytes in memory | state\|method | 47 |
| 492 | Mixed Precision | Mixed precision | Using both single and double precision in a calculation | state\|method | 8 |
| 493 | Static Linking | Static linking | The process of copying all library modules into the executable | process\|method | 7 |
| 494 | Neural Network Potential | Neural Network potential | A machine learning-based potential for interatomic interactions | model | 4 |
| 495 | BLAS | BLAS | A specification for a set of low-level linear algebra operations | software\|algorithm | 11 |
| 496 | LAPACK | LAPACK | A standard software library for numerical linear algebra | software\|algorithm | 8 |
| 497 | AMBER94 | AMBER94 | A specific version of the AMBER force field | model | 8 |
| 498 | AMBER96 | AMBER96 | A specific version of the AMBER force field | model | 3 |
| 499 | AMBER99 | AMBER99 | A specific version of the AMBER force field | model | 12 |
| 500 | AMBER99SB | AMBER99SB | A specific version of the AMBER force field with improved backbone parameters | model | 7 |
| 501 | AMBER99SB-ILDN | AMBER99SB-ILDN | An AMBER force field with improved side-chain torsion parameters | model | 3 |
| 502 | AMBER03 | AMBER03 | A specific version of the AMBER force field | model | 3 |
| 503 | AMBERGS | AMBERGS | A specific version of the AMBER force field | model | 3 |

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| 504 | ANTECHAMBER | ANTECHAMBER | A set of tools for generating parameters for organic molecules | software | 3 |
| 505 | GAFF | GAFF | Generalized Amber Force Field for small organic molecules | model | 5 |
| 506 | CHARMM19 | CHARMM19 | A united-atom version of the CHARMM force field | model | 1 |
| 507 | CHARMM22 | CHARMM22 | An all-atom version of the CHARMM force field | model | 1 |
| 508 | CHARMM36 | CHARMM36 | An all-atom version of the CHARMM force field, often used for lipids | model | 4 |
| 509 | GROMOS 53a6 | GROMOS 53a6 | A specific version of the GROMOS force field | model | 1 |
| 510 | GROMOS 53a5 | GROMOS 53a5 | A specific version of the GROMOS force field | model | 1 |
| 511 | GROMOS 43a1p | GROMOS 43a1p | A modified GROMOS force field for phosphorylated residues | model | 1 |
| 512 | OPLS-AA/M | OPLS-AA/M | An all-atom version of the OPLS force field | model | 1 |
| 513 | OPLS-UA | OPLS-UA | A united-atom version of the OPLS force field | model | 1 |
| 514 | BOSS | BOSS | A program for OPLS force field simulations | software | 1 |
| 515 | MCPRO | MCPRO | A program for OPLS force field simulations | software | 1 |
| 516 | Leap-frog integrator | md | A numerical integrator for Newton's equations of motion | algorithm | 11 |
| 517 | Brownian Dynamics integrator | bd | An integrator for systems where solvent is treated implicitly | algorithm | 0 |
| 518 | Steepest Descent | steep | An algorithm for energy minimization | algorithm | 11 |
| 519 | Conjugate Gradient | cg | An efficient algorithm for energy minimization | algorithm | 16 |
| 520 | L-BFGS | l-bfgs | A quasi-Newtonian method for energy minimization | algorithm | 10 |
| 521 | Center of Mass Motion Removal | comm-mode | A procedure to keep the system's center of mass stationary | process\|method | 12 |
| 522 | Shell Molecular Dynamics | Shell Molecular Dynamics | A model for polarizability using fictitious charged shell particles | model\|method | 3 |
| 523 | Verlet buffer | verlet-buffer-tolerance | A tolerance for pair list generation in the Verlet scheme | measure\|unit | 36 |
| 524 | Reaction Field | Reaction-Field | A method to approximate long-range electrostatics using a dielectric continuum | model\|method | 14 |
| 525 | Van der Waals interactions | Van der Waals | Weak intermolecular forces including dispersion and repulsion | model | 14 |
| 526 | Lennard-Jones potential | LJ | A simple mathematical model for Van der Waals interactions | model | 7 |
| 527 | Andersen thermostat | andersen | A thermostat that maintains temperature by random collisions | algorithm\|model | 3 |
| 528 | v-rescale thermostat | v-rescale | A velocity-rescaling thermostat with a stochastic term | algorithm\|model | 5 |
| 529 | Parrinello-Rahman barostat | Parrinello-Rahman | A barostat that allows the simulation box to change shape | algorithm\|model | 5 |
| 530 | MTTK barostat | MTTK | Martyna-Tuckerman-Tobias-Klein barostat implementation | algorithm\|model | 2 |
| 531 | Simulated Annealing | Simulated annealing | A method for finding the global minimum by slowly cooling the system | method\|algorithm | 11 |
| 532 | Velocity generation | gen-vel | The process of assigning initial velocities to atoms | process | 1 |
| 533 | Maxwell distribution | Maxwell distribution | A probability distribution for the speeds of particles in a gas | model | 2 |
| 534 | Umbrella sampling | umbrella | An enhanced sampling technique using a biasing potential | method\|algorithm | 10 |
| 535 | NMR refinement | disre | Using experimental NMR data to restrain a simulation | method | 1 |
| 536 | Free energy calculations | free-energy | Methods to compute free energy differences between states | method | 33 |
| 537 | Soft-core potentials | sc-function | Modified potentials to avoid singularities during alchemical transformations | model | 7 |
| 538 | Simulated Tempering | simulated-tempering | An enhanced sampling method where temperature is a dynamic variable | method\|algorithm | 7 |
| 539 | Non-equilibrium MD | Non-equilibrium MD | Simulations where the system is not in thermodynamic equilibrium | method\|process | 3 |

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| 540 | Multi-simulation | multidir | Running multiple related simulations in a single mdrun invocation | process\|software | 20 |
| 541 | Thread pinning | thread affinity (pinning) | Binding a software thread to a specific hardware core | process\|method | 0 |
| 542 | Hybrid/heterogeneous acceleration | Hybrid/heterogeneous acceleration | Distributing computational work between CPUs and GPUs | method\|process | 1 |
| 543 | Intra-core parallelization | Intra-core parallelization via SIMD | Using SIMD instructions to perform multiple operations in a single core | method | 2 |
| 544 | Node level parallelization | Node level parallelization | Parallelizing a simulation across multiple compute nodes | method\|process | 1 |
| 545 | Process(-or) level parallelization | Process(-or) level parallelization via OpenMP | Using OpenMP for multi-threading on a single processor | method\|process | 1 |
| 546 | Dynamic load balancing | dynamic load balancing | A technique to distribute computation evenly across processors during a run | algorithm\|method | 27 |
| 547 | Multi-level parallelization | Multi-level parallelization | Using a combination of MPI and OpenMP for parallel simulations | method | 3 |
| 548 | Thread-MPI | thread-MPI | GROMACS's internal implementation of MPI for single-node parallelism | software\|method | 65 |
| 549 | Particle-Particle (PP) ranks | PP ranks | MPI ranks that compute short-range particle-particle interactions | process\|state | 1 |
| 550 | PME ranks | PME ranks | MPI ranks dedicated to computing the long-range PME part of interactions | process\|state | 45 |
| 551 | Wallcycle module | Wallcycle module | A module for runtime performance measurement in GROMACS | software | 1 |
| 552 | GPU-resident mode | GPU-resident | A parallelization mode where force and coordinate data remain on the GPU | method\|state | 8 |
| 553 | Force-offload mode | force-offload | A parallelization mode where forces are computed on the GPU and integration on the CPU | method\|state | 3 |
| 554 | Quasiharmonic analysis | Quasiharmonic formula | A method to estimate conformational entropy from a covariance matrix | method | 0 |
| 555 | Schlitter's formula | Schlitter's formula | An alternative formula for estimating conformational entropy | method | 0 |
| 556 | Luzar & Chandler kinetics | Luzar & Chandler kinetics | A method for analyzing the kinetics of hydrogen bond formation and breaking | method | 1 |
| 557 | Dihedral correlation function | dihedral correlation function | A function that measures the time correlation of dihedral angles | measure | 1 |
| 558 | Chandler correlation function | Chandler correlation function | A function used to analyze transitions between dihedral rotamers | measure | 1 |
| 559 | Friction tensor | friction_tensor | A tensor describing the frictional forces experienced by a particle | model\|measure | 5 |
| 560 | Relative entropy | relative entropy | A measure of the 'distance' between two probability distributions | measure | 6 |
| 561 | gmx bundle | gmx bundle | A GROMACS tool for analyzing bundles of axes, such as in helices | software | 7 |
| 562 | Karplus equation | Karplus equation | An equation that relates dihedral angles to NMR J-coupling constants | model | 1 |
| 563 | Rotamers | rotamer | Conformational isomers that differ by rotation about a single bond | state | 6 |
| 564 | NUMA (Non-Uniform Memory Access) | non-uniform memory access (NUMA) | A memory design where access time depends on memory location relative to a processor | model | 0 |
| 565 | Wait GPU NB local | Wait GPU NB local | A performance counter indicating CPU is waiting for GPU non-bonded calculations | state\|measure | 1 |
| 566 | mpirun | mpirun | A common command to launch MPI parallel jobs | software | 27 |
| 567 | Rhombic dodecahedron | rhombic dodecahedron | A space-filling unit cell shape that is more spherical than a cube | model | 10 |
| 568 | Virtual interaction sites | virtual interaction sites | Fictitious particles used to represent charge distributions or lone pairs | model | 14 |
| 569 | Residue topology database | .rtp | A database file containing residue definitions for pdb2gmx | data format\|data source | 1 |
| 570 | Hydrogen-bond database | .hdb | A database file defining hydrogen bond donors and acceptors | data format\|data source | 0 |
| 571 | Counter-ions | counter-ions | Ions added to a simulation to neutralize the total charge of the system | chemical entity | 4 |
| 572 | Blowing up | blowing up | A term for a simulation that becomes numerically unstable and crashes | state | 14 |
| 573 | gmx-gangle | gmx-gangle | A GROMACS tool to calculate angles | software | 1 |

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| 574 | gmx-convert-trj | gmx-convert-trj | A GROMACS tool to convert between trajectory file formats | software | 1 |
| 575 | gmx-distance | gmx-distance | A GROMACS tool to calculate distances between pairs of positions | software | 1 |
| 576 | gmx-dssp | gmx-dssp | A GROMACS tool to calculate secondary structure using the DSSP algorithm | software | 1 |
| 577 | gmx-filter | gmx-filter | A GROMACS tool to filter trajectories | software | 1 |
| 578 | gmx-dump | gmx-dump | A GROMACS tool to make binary files human-readable | software | 1 |
| 579 | gmx-dyecoupl | gmx-dyecoupl | A GROMACS tool to extract dye dynamics from trajectories | software | 1 |
| 580 | gmx-dielectric | gmx-dielectric | A GROMACS tool to calculate frequency-dependent dielectric constants | software | 1 |
| 581 | gmx-dipoles | gmx-dipoles | A GROMACS tool to compute the total dipole moment | software | 1 |
| 582 | Single linkage | single linkage | A clustering method that adds a structure to a cluster based on its distance to any element | algorithm | 2 |
| 583 | Jarvis-Patrick | Jarvis-Patrick | A clustering method based on shared nearest neighbors | algorithm | 2 |
| 584 | Monte Carlo clustering | monte-carlo | A clustering method that reorders an RMSD matrix using Monte Carlo | algorithm | 1 |
| 585 | RMSD matrix diagonalization | diagonalization | A method to find eigenvectors and eigenvalues of the RMSD matrix | method | 1 |
| 586 | gmx clustsize | gmx clustsize | A GROMACS tool to compute size distributions of molecular/atomic clusters | software | 6 |
| 587 | gmx confrms | gmx confrms | A GROMACS tool to compute the RMSD between two structures after fitting | software | 6 |
| 588 | Mass-weighted fitting | mw | A least-squares fitting procedure where atom positions are weighted by their mass | method | 1 |
| 589 | B-factors | bfac | Values stored in PDB files, often used to represent atomic fluctuations (MSD) | measure | 10 |
| 590 | Linear Interaction Energy (LIE) | LIE (Linear Interaction Energy) method | A method for estimating binding free energies | method | 0 |
| 591 | Undulatory fluctuations | undulatory fluctuations | Wave-like motions in large lipid bilayers | process\|state | 1 |
| 592 | gmx densmap | gmx densmap | A GROMACS tool to compute 2D number-density maps | software | 6 |
| 593 | Cole-Cole plot | Cole-Cole plot | A plot of the imaginary versus the real part of the dielectric permittivity | method | 1 |
| 594 | Kirkwood G-factor | Kirkwood G-factor | A factor that relates the dielectric constant to molecular dipole correlations | measure | 1 |
| 595 | Einstein-Helfand method | Einstein-Helfand method | A method to calculate transport coefficients like viscosity and conductivity | method | 1 |
| 596 | gmx current | gmx current | A GROMACS tool for calculating current autocorrelation and dielectric constants | software | 7 |
| 597 | gmx dos | gmx dos | A GROMACS tool to compute the Density of States from velocity data | software | 11 |
| 598 | Vibrational power spectrum | vibrational power spectrum | The Fourier transform of the velocity autocorrelation function | measure | 1 |
| 599 | DSSP algorithm | DSSP algorithm | An algorithm to assign secondary structure to proteins from atomic coordinates | algorithm | 8 |
| 600 | Alpha-helix | alpha-helix | A common secondary structure motif in proteins | chemical entity | 4 |
| 601 | Beta-bridge | beta-bridge | An isolated pair of hydrogen-bonded residues forming a small beta-sheet | chemical entity | 1 |
| 602 | Extended strand | extended strand | A stretch of polypeptide chain in a beta-sheet conformation | chemical entity | 1 |
| 603 | 3_10-helix | 3_10-helix | A type of helical secondary structure in proteins | chemical entity | 1 |
| 604 | Pi-helix | pi-helix | A type of helical secondary structure in proteins | chemical entity | 1 |
| 605 | Kappa-helix | kappa-helix | A type of helical secondary structure, also known as poly-proline II helix | chemical entity | 1 |
| 606 | Hydrogen-bonded turn | hydrogen-bonded turn | A region where the polypeptide chain reverses direction, stabilized by a hydrogen bond | chemical entity | 1 |
| 607 | FRET (Förster Resonance Energy Transfer) | (F)RET simulations | A mechanism describing energy transfer between two light-sensitive molecules | process\|model | 0 |
| 608 | Foerster radius | Foerster radius | The distance at which FRET efficiency is 50% | measure | 2 |
| 609 | Triclinic box | triclinic | A simulation box defined by three vectors of arbitrary length and orientation | model | 8 |

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| 610 | Dodecahedron box | dodecahedron | A rhombic dodecahedron-shaped simulation box | model | 0 |
| 611 | Octahedron box | octahedron | A truncated octahedron-shaped simulation box | model | 0 |
| 612 | MEAD electrostatics program | MEAD electrostatics program | A program for solving the Poisson-Boltzmann equation | software | 1 |
| 613 | gmx eneconv | gmx eneconv | A GROMACS tool to concatenate and modify energy files | software | 8 |
| 614 | gmx enemat | gmx enemat | A GROMACS tool to extract an energy matrix from an energy file | software | 8 |
| 615 | Heat capacity | Heat capacity C_p | A measure of the heat energy required to raise the temperature of a substance | measure | 12 |
| 616 | Thermal expansion coefficient | Thermal expansion coeff. | A measure of the fractional change in volume per degree change in temperature | measure | 0 |
| 617 | Isothermal compressibility | Isothermal compressibility | A measure of the relative volume change in response to a pressure change | measure | 4 |
| 618 | Adiabatic bulk modulus | Adiabatic bulk modulus | A measure of a substance's resistance to compression under adiabatic conditions | measure | 1 |
| 619 | gmx extract-cluster | gmx extract-cluster | A GROMACS tool to extract trajectory frames corresponding to clusters | software | 9 |
| 620 | Frequency filtering | frequency filtering | A method to remove high or low-frequency motions from a trajectory | method | 2 |
| 621 | gmx freevolume | gmx freevolume | A GROMACS tool to calculate the free volume in a system | software | 7 |
| 622 | Fractional Free Volume (FFV) | Fractional Free Volume (FFV) | The fraction of the volume not occupied by the hard-sphere atoms | measure | 1 |
| 623 | gmx genconf | gmx genconf | A GROMACS tool to generate multiple copies of a molecule in a grid | software | 9 |
| 624 | Distance restraints | disre_dist | Restraints used to enforce a specific distance between atoms | model | 31 |
| 625 | Freezing atoms | freeze | Completely immobilizing a group of atoms during a simulation | method | 1 |
| 626 | Maxwellian distribution | Maxwellian distribution | A probability distribution for particle speeds at a given temperature | model | 1 |
| 627 | gmx vanhove | gmx vanhove | A GROMACS tool to compute the Van Hove correlation function | software | 10 |
| 628 | Van Hove correlation function | Van Hove correlation function | The probability of finding a particle at position r at time t, given it was at r0 at t=0 | measure | 1 |
| 629 | Momentum autocorrelation function | momentum autocorrelation function | The autocorrelation function of the total momentum of a group of atoms | measure | 2 |
| 630 | Weighted Histogram Analysis Method (WHAM) | Weighted Histogram Analysis Method (WHAM) | A method to compute a potential of mean force from a series of biased simulations | method\|algorithm | 1 |
| 631 | Potential of Mean Force (PMF) | potential of mean force (PMF) | The free energy profile along a reaction coordinate | measure\|model | 3 |
| 632 | Integrated autocorrelation time (IACT) | integrated autocorrelation time (IACT) | A measure of the statistical inefficiency in a time series | measure | 1 |
| 633 | Bootstrap analysis | bootstrap analysis | A statistical method for estimating the uncertainty of an estimator | method | 1 |
| 634 | gmx x2top | gmx x2top | A GROMACS tool to generate a primitive topology from a coordinate file | software | 12 |
| 635 | XPixelMap (.xpm) | XPixelMap file | A file format for storing image data as an array of characters | data format | 0 |
| 636 | gmx wrapper binary | gmx wrapper | The main GROMACS executable that provides access to all the individual tools | software | 3 |
| 637 | Selection syntax | Selection syntax | The language used in GROMACS to select atoms for analysis | method | 8 |
| 638 | Center of mass (COM) | com of | The average position of all the atoms in a group, weighted by mass | measure | 1 |
| 639 | Center of geometry (COG) | cog of | The average position of all the atoms in a group, without mass weighting | measure | 0 |
| 640 | Solid angle | insolidangle | A measure of how large an object appears to an observer looking from a single point | measure | 4 |
| 641 | g_bond | g_bond | A legacy GROMACS tool for calculating distances, replaced by gmx distance | software | 3 |
| 642 | g_dist | g_dist | A legacy GROMACS tool for calculating distances, replaced by gmx distance and gmx select | software | 4 |
| 643 | g_sgangle | g_sgangle | A legacy GROMACS tool for calculating angles, replaced by gmx gangle | software | 4 |
| 644 | gmx protonate | gmx protonate | A legacy GROMACS tool for adding protons to a structure | software | 1 |

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| 645 | g_sas | g_sas | A legacy GROMACS tool for calculating solvent accessible surface area, replaced by gmx sasa | software | 1 |
| 646 | genbox | genbox | A legacy GROMACS tool for solvation, split into gmx solvate and gmx insert-molecules | software | 4 |
| 647 | tpbconv | tpbconv | A legacy GROMACS tool for converting run input files, renamed to gmx convert-tpr | software | 1 |
| 648 | Equipartition theorem | equipartition theorem | A theorem that relates the temperature of a system to its average kinetic energy | model | 1 |
| 649 | Hot-solvent/cold-solute problem | hot-solvent/cold-solute problem | An artifact that can arise when using separate thermostats for solute and solvent | state | 0 |
| 650 | Energy conservation | Energy conservation | The principle that the total energy of an isolated system remains constant | model | 9 |
| 651 | Round-off error | Round-off error | The difference between an exact value and its floating-point representation | measure | 1 |
| 652 | Average structure | Average structure | A structure obtained by averaging the atomic coordinates over a trajectory | model | 13 |
| 653 | Steric clashes | steric clashes | Unfavorable interactions that occur when atoms are too close to each other | state | 1 |
| 654 | NVE ensemble | NVE | A statistical ensemble with constant number of particles, volume, and energy | model\|state | 0 |
| 655 | Environment Variables | Environment Variables | Variables that can be set in the shell to influence the behavior of GROMACS programs | software | 51 |
| 656 | Floating point arithmetic | Floating point arithmetic | The arithmetic used by computers to represent and operate on real numbers | method | 4 |
| 657 | Binary floating-point | binary floating-point | A representation of real numbers using a binary base | method | 2 |
| 658 | E notation | E notation | A computer form of scientific notation for floating-point numbers | method | 1 |
| 659 | Deprecating functionality | Policy for deprecating GROMACS functionality | The process of marking old features for future removal | process | 0 |
| 660 | gmx-help | gmx-help | A GROMACS tool to print help information | software | 0 |
| 661 | Maxwell-Boltzmann distribution | Maxwell-Boltzmann distribution | A probability distribution for particle speeds at a given temperature | model | 2 |
| 662 | Langevin dynamics | Langevin dynamics | A mathematical description of stochastic dynamics | model | 4 |
| 663 | Dissipative Particle Dynamics (DPD) | dissipative particle dynamics (DPD) | A coarse-grained simulation method that includes hydrodynamic interactions | method\|model | 0 |
| 664 | Brownian Dynamics | Brownian Dynamics | A simplified form of Langevin dynamics for over-damped systems | method\|algorithm | 9 |
| 665 | Position Langevin dynamics | position Langevin dynamics | Another name for Brownian dynamics | method\|algorithm | 2 |
| 666 | L-BFGS minimizer | L-BFGS minimizer | A quasi-Newton method for energy minimization | algorithm | 1 |
| 667 | Slow-growth method | Slow-growth methods | A method for free energy calculation by slowly changing the Hamiltonian | method | 0 |
| 668 | Thermodynamic cycle | thermodynamic cycle | A cycle of thermodynamic processes used to calculate state function changes | model | 1 |
| 669 | Helmholtz free energy | Helmholtz free energy | A thermodynamic potential that measures useful work obtainable from a closed system | measure | 2 |
| 670 | Gibbs free energy | Gibbs free energy | A thermodynamic potential that measures the maximum reversible work from a system | measure | 2 |
| 671 | MBAR (Multistate Bennett Acceptance Ratio) | MBAR | An extension of BAR for multiple states | method\|algorithm | 0 |
| 672 | Replica exchange molecular dynamics (REMD) | Replica exchange molecular dynamics (REMD) | A method to enhance sampling by exchanging temperatures between replicas | method\|algorithm | 1 |
| 673 | Hamiltonian replica exchange | Hamiltonian replica exchange | A variant of REMD where Hamiltonians are exchanged instead of temperatures | method\|algorithm | 2 |
| 674 | Gibbs sampling replica exchange | Gibbs sampling replica exchange | A replica exchange method where all possible pairs are tested for exchange | method\|algorithm | 4 |
| 675 | Expanded Ensemble simulation | Expanded Ensemble simulation | A simulation method that samples both coordinates and thermodynamic states | method\|algorithm | 2 |
| 676 | Half-shell method | half-shell method | A method for assigning forces in domain decomposition | method | 1 |

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| 677 | Eighth shell method | eighth shell method | A communication-efficient method for assigning forces in domain decomposition | method | 1 |
| 678 | Midpoint method | midpoint method | An alternative communication-efficient method for assigning forces | method | 3 |
| 679 | Pencil decomposition | pencil decomposition | A 2-D domain decomposition strategy for PME calculations | algorithm\|method | 1 |
| 680 | Multiple-Program, Multiple-Data (MPMD) | Multiple-Program, Multiple-Data PME parallelization | A parallelization scheme where some ranks only perform PME calculations | method | 0 |
| 681 | Pair-additive force field | pair-additive | A force field where non-bonded interactions are a sum of pairwise terms | model | 0 |
| 682 | Lorentz-Berthelot rules | Lorentz-Berthelot rules | Combination rules for calculating cross-interaction Lennard-Jones parameters | model | 2 |
| 683 | Combination rules | combination rules | Rules to determine interaction parameters between different atom types | model | 23 |
| 684 | Reaction-field electrostatics | Coulomb interaction with reaction field | A method to treat long-range electrostatics by embedding the system in a dielectric continuum | model\|method | 4 |
| 685 | Force-switch function | force-switch function | A function that smoothly switches the force to zero at the cutoff | model\|method | 1 |
| 686 | Potential-switch function | potential-switch function | A function that smoothly switches the potential to zero at the cutoff | model\|method | 1 |
| 687 | Fourth power potential | Fourth power potential | A bond stretching potential used in the GROMOS-96 force field | model | 2 |
| 688 | FENE potential | FENE bond stretching potential | A finitely extensible nonlinear elastic potential for coarse-grained polymers | model | 0 |
| 689 | Bond-Bond cross term | Bond-Bond cross term | A potential term coupling the stretching of two adjacent bonds | model | 2 |
| 690 | Bond-Angle cross term | Bond-Angle cross term | A potential term coupling bond stretching and angle bending | model | 2 |
| 691 | Improper dihedrals | Improper dihedrals | Dihedral terms used to maintain planarity or chirality | model | 15 |
| 692 | Ryckaert-Bellemans potential | Ryckaert-Bellemans function | A dihedral potential expressed as a power series in cos(phi) | model | 4 |
| 693 | Fourier function (dihedral) | Fourier function | A dihedral potential expressed as a Fourier series | model | 0 |
| 694 | Restricted torsion potential | Restricted torsion potential | A dihedral potential that prevents full rotation | model | 1 |
| 695 | Tabulated bonded interactions | Tabulated bonded interaction functions | User-defined potentials for bonded interactions read from a table | model | 3 |
| 696 | Flat-bottomed position restraints | Flat-bottomed position restraints | Restraints that act only when a particle moves outside a defined region | model | 6 |
| 697 | Angle restraints | Angle restraints | Restraints applied to the angle between vectors | model | 3 |
| 698 | Time averaging (restraints) | Time averaging | Using a time-averaged distance for restraints instead of the instantaneous distance | method | 0 |
| 699 | Ensemble averaging (restraints) | Ensemble averaging | Averaging restraints over multiple simulated subsystems | method | 0 |
| 700 | Drude particles | Drude particles | Shell particles used in polarizable force fields | model | 0 |
| 701 | Thole polarization | Thole polarization | A model for screening intramolecular electrostatic interactions in polarizable systems | model | 1 |
| 702 | Soft-core interactions | Soft-core interactions | Modified potentials used in free energy calculations to avoid singularities | model | 10 |
| 703 | Gapsys soft-core | Gapsys et al. | A specific functional form for soft-core interactions | model | 1 |
| 704 | Trotter decomposition | Trotter decomposition | A mathematical method to approximate the evolution operator in simulations | method | 7 |
| 705 | Wiener process | Wiener process | A mathematical model for Brownian motion, used in stochastic thermostats | model | 1 |
| 706 | Nosé-Hoover chain | Nosé-Hoover chain | An extension of the Nosé-Hoover thermostat to improve ergodicity | algorithm\|model | 4 |
| 707 | Stochastic cell rescaling | Stochastic cell rescaling | A barostat that includes a stochastic term to ensure correct volume fluctuations | algorithm\|model | 9 |
| 708 | Surface-tension coupling | Surface-tension coupling | A pressure coupling scheme for systems with interfaces | method\|model | 1 |
| 709 | RATTLE | RATTLE | An algorithm for constraining velocities in velocity Verlet integration | algorithm | 3 |
| 710 | Holonomic constraints | holonomic constraints | Constraints that depend only on the coordinates of the particles | model | 3 |

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| 711 | Lagrange multipliers | Lagrange multipliers | Variables introduced to solve constrained optimization problems | method | 4 |
| 712 | PRODRG | PRODRG | A server for generating topologies and coordinates for small molecules | software | 1 |
| 713 | PyMOL | PyMOL | A molecular visualization system | software | 3 |
| 714 | Rasmol | Rasmol | A molecular graphics program for visualizing macromolecules | software | 10 |
| 715 | Protein Explorer | Protein Explorer | A web-based tool for macromolecular structure exploration | software | 2 |
| 716 | Chimera | Chimera | A program for interactive visualization and analysis of molecular structures | software | 2 |
| 717 | Molscript | Molscript | A program for creating schematic or detailed 3D representations of molecules | software | 1 |
| 718 | LOOS | LOOS | A C++ library for analyzing molecular dynamics trajectories | software | 1 |
| 719 | MDAnalysis | MDAnalysis | A Python library for the analysis of molecular dynamics simulations | software | 1 |
| 720 | MDTraj | MDTraj | A Python library for analyzing molecular dynamics trajectories | software | 1 |
| 721 | Pteros | Pteros | A C++ library for structural bioinformatics and molecular simulations | software | 1 |
| 722 | Grace | Grace | A 2D plotting tool for the X Window System | software | 16 |
| 723 | gnuplot | gnuplot | A command-line driven graphing utility | software | 3 |
| 724 | Matplotlib | Matplotlib | A plotting library for the Python programming language | software | 2 |
| 725 | Micelle Clustering | Micelle Clustering | A process to ensure a micelle is not split across periodic boundaries | process | 4 |
| 726 | CODATA | CODATA | The Committee on Data for Science and Technology, a source for fundamental physical constants | data source | 2 |
| 727 | NIST | NIST | The National Institute of Standards and Technology, a source for physical constants | data source | 1 |
| 728 | ps | ps | Picosecond, a unit of time | unit | 349 |
| 729 | e | e | The elementary charge, a unit of electric charge | unit | 797 |
| 730 | u | u | The unified atomic mass unit, a unit of mass | unit | 56 |
| 731 | bar | bar | A unit of pressure | unit | 62 |
| 732 | Debye | Debye | A unit of electric dipole moment | unit | 6 |
| 733 | V/m | Vm-1 | Volts per meter, a unit of electric field strength | unit | 0 |
| 734 | kcal/mol | kcal mol-1 | Kilocalories per mole, a unit of energy | unit | 1 |
| 735 | Angstrom | Å | Angstrom, a unit of length (0.1 nm) | unit | 0 |
| 736 | fs | fs | Femtosecond, a unit of time | unit | 52 |
| 737 | ns | ns | Nanosecond, a unit of time | unit | 43 |
| 738 | us | us | Microsecond, a unit of time | unit | 64 |
| 739 | ms | ms | Millisecond, a unit of time | unit | 34 |
| 740 | s | s | Second, a unit of time | unit | 466 |
| 741 | degrees | degrees | A unit of angle measurement | unit | 91 |
| 742 | radians | rad | A unit of angle measurement | unit | 5 |
| 743 | kJ/mol/rad^2 | kJ/mol/rad^2 | A unit for an angular force constant | unit | 2 |
| 744 | nm/ps | nm/ps | A unit of velocity | unit | 3 |
| 745 | deg/ps | deg/ps | A unit of angular velocity | unit | 1 |
| 746 | nm^2/ps | nm^2/ps | A unit for a diffusion constant | unit | 0 |

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| 747 | rad^2/ps | rad^2/ps | A unit for a rotational diffusion constant | unit | 0 |
| 748 | amu/ps | amu/ps | A unit for a friction coefficient | unit | 1 |
| 749 | nm^3 | nm-3 | A unit for number density | unit | 3 |
| 750 | nm^-2 | nm-2 | A unit for surface number density | unit | 0 |
| 751 | 1/nm | 1/nm | A unit for the scattering vector q | unit | 9 |
| 752 | 1/cm | 1/cm | Wavenumber, a unit of frequency | unit | 2 |
| 753 | Hz | Hz | Hertz, a unit of frequency | unit | 4 |
| 754 | D | D | Debye, a unit of electric dipole moment | unit | 173 |
| 755 | kT | kT | A unit of energy, Boltzmann's constant times temperature | unit | 25 |
| 756 | kJ/mol/nm^4 | kcal/mol/nm4 | A unit for the khyp force constant in anharmonic polarization | unit | 0 |
| 757 | nm/e^2 | nm/e^2 | A unit for the alphaQ parameter in Gapsys soft-core potentials | unit | 1 |
| 758 | bar^-1 | bar-1 | Inverse bar, a unit of compressibility | unit | 0 |
| 759 | V nm^-1 | V nm-1 | A unit for electric field strength | unit | 0 |
| 760 | ps^-1 | ps-1 | Inverse picosecond, a unit of frequency or friction | unit | 0 |
| 761 | kJ/mol/nm | kJ/mol nm | A unit for force | unit | 2 |
| 762 | kJ/mol/rad | kJ/mol rad | A unit for torque | unit | 2 |
| 763 | nm/step | nm/step | A unit for stepsize in linear expansion | unit | 3 |
| 764 | keV | keV | Kilo-electronvolt, a unit of energy for X-rays | unit | 1 |
| 765 | Virtual site | rs | A point with constructed coordinates from other atoms | model\|chemical entity | 78 |
| 766 | Linear combination of two atoms | | A method to construct a virtual site | model\|method | 1 |
| 767 | Fixed distance virtual site | 2fd | Virtual site on a line through two atoms | model\|method | 0 |
| 768 | Linear combination of three atoms | | A method to construct a virtual site in a plane | model\|method | 2 |
| 769 | Fixed distance in plane virtual site | 3fd | Virtual site in a plane of three atoms | model\|method | 0 |
| 770 | Fixed angle and distance in plane virtual site | 3fad | Virtual site in a plane with fixed angle/distance | model\|method | 0 |
| 771 | Out of plane non-linear combination | 3out | Virtual site constructed out of the plane of three atoms | model\|method | 0 |
| 772 | Fixed distance from four atoms virtual site | 4fdn | A stable virtual site construction from four atoms | model\|method | 0 |
| 773 | Virtual site source code | vsite.c | The source code file implementing virtual site calculations | data source\|software | 0 |
| 774 | Center of geometry | center of geometry | A method for setting weights in virtual site construction | method\|model | 3 |
| 775 | Center of mass | center of mass | A method for setting weights using atomic masses | method\|model | 102 |
| 776 | Center of weights | center of weights | A method for setting weights using user-defined values | method\|model | 1 |
| 777 | Long Range Electrostatics | Long Range Electrostatics | Methods for calculating electrostatic interactions over long distances | method\|model | 3 |
| 778 | Direct space sum | Vdir | The direct space component of the Ewald summation | measure\|model | 2 |

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| 779 | Reciprocal space sum | Vrec | The reciprocal space component of the Ewald summation | measure\|model | 2 |
| 780 | Ewald splitting parameter | ? | Determines the weight between direct and reciprocal sums | measure | 0 |
| 781 | GROMACS run parameter file | mdp | File containing parameters for a GROMACS simulation run | data format | 0 |
| 782 | Coulomb interaction type | coulombtype | Parameter to select the method for electrostatic interactions | identifier\|model | 0 |
| 783 | Van der Waals cutoff radius | rvdw | Cutoff distance for van der Waals interactions | measure | 0 |
| 784 | Neighbor list cutoff | rlist | Cutoff distance for generating the neighbor list | measure | 0 |
| 785 | Coulomb cutoff | rcoulomb | Cutoff distance for Coulomb interactions in the direct space | measure | 1 |
| 786 | Fourier spacing | fourierspacing | Grid spacing for the reciprocal space part of PME/Ewald | measure | 1 |
| 787 | Ewald relative tolerance | ewald-rtol | Relative strength of the electrostatic interaction at the cutoff | measure | 1 |
| 788 | Cardinal B-spline interpolation | cardinal B-spline interpolation | Interpolation method used in the PME algorithm | algorithm\|method | 1 |
| 789 | Smooth PME | SPME | GROMACS implementation of PME using smooth B-splines | algorithm\|method | 3 |
| 790 | Verlet cut-off scheme | Verlet cut-off scheme | A cutoff scheme where the potential is unmodified | method\|model | 5 |
| 791 | PME interpolation order | pme-order | Controls the interpolation order in the PME method | measure | 0 |
| 792 | Long Range Van der Waals interactions | Long Range Van der Waals interactions | Methods to account for VdW interactions beyond the cutoff | method\|model | 2 |
| 793 | Dispersion interaction parameter | C6 | Coefficient for the r?? term in the Lennard-Jones potential | measure | 0 |
| 794 | Long-range dispersion energy | Vlr | The energy contribution from dispersion interactions beyond the cutoff | measure | 0 |
| 795 | Radial distribution function | g(r) | Describes the probability of finding a particle at a distance r | measure | 6 |
| 796 | Average dispersion constant | ?C6? | Average C6 parameter for a homogeneous mixture | measure | 2 |
| 797 | Pressure | P | A thermodynamic property of the system | measure\|state | 268 |
| 798 | Long-range virial correction | ?lr | Correction to the virial due to truncated interactions | measure | 0 |
| 799 | Long-range pressure correction | Plr | Correction to the pressure due to truncated interactions | measure | 0 |
| 800 | Lennard-Jones PME | Lennard-Jones PME | Application of the PME method to Lennard-Jones interactions | algorithm\|method | 1 |
| 801 | Geometrically combined dispersion parameter | C?,geom | Dispersion parameter from geometric mean of individual parameters | measure\|model | 0 |
| 802 | Lorentz-Berthelot combination rules | Lorentz-Berthelot combination rules | Rules for combining Lennard-Jones parameters for unlike atoms | model\|method | 3 |
| 803 | Direct space dispersion parameter | Cdir | Dispersion parameter used in the direct space calculation | measure | 0 |
| 804 | Reciprocal space dispersion parameter | Crecip | Dispersion parameter used in the reciprocal space calculation | measure | 0 |
| 805 | VdW interaction modifier | vdw-modifier | Modifies the van der Waals potential at the cutoff | method\|model | 1 |
| 806 | Potential-shift modifier | Potential-Shift | A VdW modifier that shifts the potential to be zero | model\|method | 0 |
| 807 | LJ-PME relative tolerance | ewald-rtol-lj | Tolerance for splitting direct and reciprocal space in LJ-PME | measure | 0 |
| 808 | LJ-PME combination rule | lj-pme-comb-rule | Combination rule for the reciprocal part of LJ-PME | identifier\|model | 0 |
| 809 | GROMOS-96 force field | GROMOS-96 | A specific united-atom force field for biomolecular simulation | model\|data source | 8 |
| 810 | OPLS-AA/L force field | OPLS-AA/L | A specific all-atom force field for biomolecular simulation | model\|data source | 0 |
| 811 | Twin-range cut-off | twin-range cut-off | A cutoff scheme with two different cutoff distances | method\|model | 3 |

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| 812 | GROMOS-87 force field | GROMOS-87 | An older version of the GROMOS force field | model\|data source | 3 |
| 813 | Fourth power bond stretching potential | Fourth power bond stretching potential | A potential energy function for bond stretching | model | 1 |
| 814 | Cosine based angle potential | Cosine based angle potential | A potential energy function for angle bending | model | 2 |
| 815 | GROMOS-96 file format | g96 | Coordinate and trajectory file format for GROMOS-96 | data format | 0 |
| 816 | Correction Map | CMAP | Energy correction maps for protein backbone dihedral angles | model\|method | 2 |
| 817 | Disable CMAP option | -nocmap | Command-line option to disable the use of CMAPs | identifier | 0 |
| 818 | CMAP types directive | [ cmaptypes ] | Topology file section defining CMAP parameters | data format | 0 |
| 819 | Residue topology parameter file | rtp file | File containing residue-specific topology information | data format | 1 |
| 820 | Coarse-graining | Coarse-graining | A method to simplify a system by grouping atoms | method\|model | 5 |
| 821 | MARTINI force field | MARTINI force field | A popular coarse-grained force field for biomolecular systems | model\|data source | 2 |
| 822 | Iterative Boltzmann inversion | iterative Boltzmann inversion | A method to derive coarse-grained potentials from distribution functions | algorithm\|method | 0 |
| 823 | Inverse Monte Carlo | Inverse Monte Carlo | A method to derive coarse-grained potentials | algorithm\|method | 1 |
| 824 | Force matching | Force matching | A method to derive coarse-grained potentials by matching forces | algorithm\|method | 1 |
| 825 | VOTCA software | VOTCA | A software package for systematic coarse-graining | software | 0 |
| 826 | PLUM force field | PLUM force field | A coarse-grained solvent-free model for protein-membrane systems | model\|data source | 1 |
| 827 | GROMACS trajectory file | trr | GROMACS file format for full precision trajectories | data format | 0 |
| 828 | Particle Type | Particle type | Defines if a particle is an atom, shell, or virtual site | identifier | 4 |
| 829 | Atom Type | Atom type | A label for an atom used for force field parameter assignment | identifier\|model | 34 |
| 830 | Virtual sites directive | [ virtual_sites? ] | Topology file section for defining virtual interaction sites | data format | 0 |
| 831 | Virtual site function type | funct | Defines the rule for constructing a virtual site | identifier | 0 |
| 832 | Normalize virtual site bonds option | -normvsbds | An option for grompp related to virtual site bonds | identifier | 0 |
| 833 | Generic virtual sites directive | [ virtual_sitesn ] | A generic directive for constructing virtual sites from N atoms | data format | 0 |
| 834 | Lennard-Jones epsilon | epsilon | The well-depth parameter in the Lennard-Jones potential | measure | 0 |
| 835 | Lennard-Jones sigma | sigma | The finite distance where the Lennard-Jones potential is zero | measure | 0 |
| 836 | Atomic mass unit | a.m.u. | A unit of mass for atoms and molecules | unit | 2 |
| 837 | Elementary charge | electron | The fundamental unit of electric charge | unit | 1 |
| 838 | Non-bonded parameter file | ffnonbonded.itp | Force field file containing parameters for non-bonded interactions | data format | 0 |
| 839 | Atom types directive | [ atomtypes ] | Topology file section defining atom types and their parameters | data format | 0 |
| 840 | Non-bonded parameters directive | [ nonbond_params ] | Topology file section for non-bonded interaction parameters between different atom types | data format | 0 |
| 841 | Lennard-Jones parameters | V(c6), W(c12) | The attractive and repulsive parameters for the Lennard-Jones potential | measure | 8 |
| 842 | Combination rule | combination rule | A rule to determine interaction parameters between different atom types | model\|method | 13 |
| 843 | Defaults directive | [ defaults ] | Topology file section for setting global simulation parameters | data format | 1 |
| 844 | Bonded parameter file | ffbonded.itp | Force field file containing parameters for bonded interactions | data format | 0 |
| 845 | Bond types directive | [ bondtypes ] | Topology file section defining parameters for covalent bonds | data format | 0 |
| 846 | Angle types directive | [ angletypes ] | Topology file section defining parameters for bond angles | data format | 0 |

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| 847 | Dihedral types directive | [ dihedraltypes ] | Topology file section defining parameters for dihedral angles | data format | 0 |
| 848 | Ryckaert-Bellemans Dihedral | Ryckaert-Bellemans Dihedrals | A specific potential function for dihedral angles | model | 2 |
| 849 | Wildcard atom type | X | A symbol used in parameter files to match any atom type | identifier | 1 |
| 850 | Moleculetype directive | [ moleculetype ] | Topology file section that defines a single type of molecule | data format | 0 |
| 851 | Intermolecular interactions directive | [ intermolecular_interactions ] | Topology section for specifying special interactions between molecules | data format | 0 |
| 852 | Intramolecular pair interactions | Intramolecular pair interactions | Special non-bonded interactions within a molecule, typically 1-4 pairs | model | 2 |
| 853 | Pairs directive | [ pairs ] | Topology file section for defining intramolecular pair interactions | data format | 0 |
| 854 | Pair types directive | [ pairtypes ] | Parameter section for intramolecular pair interaction types | data format | 0 |
| 855 | Non-bonded pairs directive | [ pairs_nb ] | A directive for non-bonded pairs used in free energy calculations | data format | 0 |
| 856 | Exclusions | Exclusions | A list of atom pairs whose non-bonded interactions should be ignored | model\|method | 54 |
| 857 | Exclusions directive | [ exclusions ] | Topology file section for manually specifying excluded non-bonded interactions | data format | 0 |
| 858 | Constraints directive | [ constraints ] | Topology file section for defining distance constraints | data format | 0 |
| 859 | Settles directive | [ settles ] | A topology directive to apply the SETTLE algorithm to a molecule | data format | 0 |
| 860 | Force field ITAP file | forcefield.itp | The main include file for a GROMACS force field | data format | 0 |
| 861 | Residue types data file | residuetypes.dat | A file that classifies residue names into categories | data format | 0 |
| 862 | Bonded types directive | [ bondedtypes ] | A directive in a residue topology file for interaction types | data format | 0 |
| 863 | Impropers directive | [ impropers ] | A directive for defining improper dihedral angles | data format | 0 |
| 864 | Charge group | charge group | A group of atoms with a net integer charge | model\|chemical entity | 19 |
| 865 | Special bonds data file | specbond.dat | A file for defining non-standard covalent bonds, like disulfide bridges | data format | 0 |
| 866 | Internal GROMACS residue names | ARG, ARGN, ASP, ASPH... | Standardized residue names used internally by GROMACS | identifier\|chemical entity | 0 |
| 867 | General atom translation file | xlateat.dat | A file for translating common non-standard atom names to IUPAC/PDB convention | data source\|data format | 0 |
| 868 | Replace directive | [ replace ] | A directive in termini databases to replace an existing atom | data format | 0 |
| 869 | Add directive | [ add ] | A directive in termini databases to add new atoms | data format | 0 |
| 870 | Delete directive | [ delete ] | A directive in termini databases to delete existing atoms | data format | 0 |
| 871 | Special bonds | Special bonds | Inter-residue bonds that are not part of the polymer backbone | model | 4 |
| 872 | Constrainttype directive | [ constrainttype ] | A directive for defining constraint parameters | data format | 0 |
| 873 | G96 bond potential | G96 bond | A fourth-power bond stretching potential from GROMOS-96 | model | 0 |
| 874 | Cubic bond potential | cubic bond | A bond potential defined by a cubic function | model | 0 |
| 875 | FENE bond potential | FENE bond | A finitely extensible nonlinear elastic bond potential | model | 0 |
| 876 | Tabulated bond potential | tabulated bond | A bond potential defined by a user-supplied table | model | 0 |
| 877 | Restraint potential | restraint potential | A potential used to restrain atoms to a reference position | model | 9 |
| 878 | G96 angle potential | G96 angle | An angle potential based on the cosine of the angle | model | 0 |
| 879 | Cross bond-bond potential | cross bond-bond | A potential term coupling the stretching of two adjacent bonds | model | 0 |
| 880 | Cross bond-angle potential | cross bond-angle | A potential term coupling bond stretching and angle bending | model | 0 |
| 881 | Tabulated angle potential | tabulated angle | An angle potential defined by a user-supplied table | model | 0 |

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| 882 | Proper dihedral potential | proper dihedral | A potential function for torsion around a central bond | model | 1 |
| 883 | Improper dihedral potential | improper dihedral | A potential used to maintain planarity or chirality | model | 3 |
| 884 | Periodic improper dihedral potential | periodic improper dihedral | An improper dihedral potential with a periodic functional form | model | 0 |
| 885 | Tabulated dihedral potential | tabulated dihedral | A dihedral potential defined by a user-supplied table | model | 0 |
| 886 | Restricted dihedral potential | restricted dihedral | A potential used to restrict the rotation of a dihedral angle | model | 0 |
| 887 | N-body virtual site (COG) | N-body virtual site (COG) | A virtual site constructed at the center of geometry of N atoms | model | 1 |
| 888 | N-body virtual site (COM) | N-body virtual site (COM) | A virtual site constructed at the center of mass of N atoms | model | 1 |
| 889 | N-body virtual site (COW) | N-body virtual site (COW) | A virtual site constructed from a center of weights of N atoms | model | 1 |
| 890 | Position restraint | position restraint | A restraint that penalizes the deviation of an atom from a reference position | model\|method | 10 |
| 891 | Flat-bottomed position restraint | flat-bottomed position restraint | A position restraint with a zero-force region around the reference | model\|method | 1 |
| 892 | Distance restraint | distance restraint | A restraint that penalizes the deviation of a distance from a reference value | model\|method | 14 |
| 893 | Dihedral restraint | dihedral restraint | A restraint that penalizes the deviation of a dihedral angle from a reference value | model\|method | 0 |
| 894 | Orientation restraint | orientation restraint | A restraint that penalizes the deviation of a molecule's orientation | model\|method | 11 |
| 895 | Angle restraint | angle restraint | A restraint that penalizes the deviation of an angle from a reference value | model\|method | 1 |
| 896 | Include directive | #include | A preprocessor directive to include the contents of another file | software | 1 |
| 897 | Position restraints directive | [ position_restraints ] | Topology file section for applying position restraints to specific atoms | data format | 0 |
| 898 | Dihedral restraints directive | [ dihedral_restraints ] | Topology file section for applying restraints to specific dihedral angles | data format | 0 |
| 899 | TIP3P water model file | tip3p.itp | An include file containing the topology for the TIP3P water model | data source\|data format | 0 |
| 900 | Define directive | #define | A preprocessor directive to define a macro or a symbol | software | 0 |
| 901 | Non-bonded function type | nbfunc | Parameter specifying the non-bonded interaction function (e.g., Lennard-Jones) | identifier | 2 |
| 902 | LJ 1-4 fudge factor | fudgeLJ | A scaling factor applied to 1-4 Lennard-Jones interactions | measure | 0 |
| 903 | QQ 1-4 fudge factor | fudgeQQ | A scaling factor applied to 1-4 electrostatic interactions | measure | 0 |
| 904 | Exclusion distance | nrexcl | The number of bonds away to exclude non-bonded interactions | measure | 1 |
| 905 | Molecule include file | Molecule.itp file | An include file containing the topology for a single molecule type | data format | 0 |
| 906 | Ifdef directive | #ifdef | A preprocessor directive for conditional compilation | software | 0 |
| 907 | Define option for grompp | -D... | A command-line option for grompp to define a preprocessor symbol | identifier | 0 |
| 908 | Constraint forces | Constraint forces | The forces required to satisfy distance constraints in a system | measure | 6 |
| 909 | GROMOS96 force field versions | GROMOS96 43a1, 43a2, ... | Specific parameter sets of the GROMOS96 force field | model\|data source | 0 |
| 910 | Run parameters file | m2p | Input file for the gmx xpm2ps utility | data format | 0 |
| 911 | Protein DataBank file | pdb | A standard file format for atomic coordinates | data format | 2 |
| 912 | Portable run input file | tpr | GROMACS binary file containing the complete simulation topology and coordinates | data format | 0 |
| 913 | Atom naming definition file | n2t | A file used for simple translation of atom names to types | data format | 0 |
| 914 | Atom type library file | atp | A file containing a library of atom types | data format | 0 |
| 915 | Compressed trajectory file | tng | A portable, compressed GROMACS trajectory format | data format | 5 |
| 916 | Binary energy file | ene | A binary GROMACS file for storing energy terms | data format | 1 |

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| 917 | Portable energy file | edr | A portable GROMACS file for storing energy terms | data format | 2 |
| 918 | Generic data file | dat | A generic file format for input or output in GROMACS | data format | 25 |
| 919 | Essential dynamics input file | edi | An input file for running simulations with essential dynamics constraints | data format | 0 |
| 920 | Encapsulated Postscript file | eps | A graphics file format for plots | data format | 0 |
| 921 | Log file | log | A human-readable file that logs the progress of a GROMACS program | data format | 89 |
| 922 | Binary matrix file | mtx | A binary file format for storing matrices, such as a Hessian | data format | 0 |
| 923 | Generic output file | out | A generic file format for output from GROMACS programs | data format | 7 |
| 924 | Portable checkpoint file | cpt | A file that stores the complete state of a simulation for restarting | data format | 1 |
| 925 | Integrator | integrator | The algorithm used to advance the positions and velocities of atoms in time | identifier\|algorithm | 101 |
| 926 | Timestep | dt | The time duration of a single step in a simulation | measure | 37 |
| 927 | Number of steps | nsteps | The total number of integration steps to perform in a simulation | measure | 29 |
| 928 | Log output frequency | nstlog | The frequency (in steps) at which to write to the log file | measure | 0 |
| 929 | Compressed trajectory output frequency | nstxout-compressed | The frequency (in steps) at which to write to the compressed trajectory file | measure | 0 |
| 930 | Continuation state | continuation | A parameter indicating whether the simulation is a continuation of a previous run | state | 0 |
| 931 | VdW interaction type | vdwtype | The method used for van der Waals interactions (e.g., Cut-off) | identifier | 0 |
| 932 | Temperature coupling groups | tc-grps | The groups of atoms that are coupled to separate thermostats | identifier | 3 |
| 933 | Temperature coupling time constant | tau-t | The time constant for the thermostat | measure | 1 |
| 934 | Reference temperature | ref-t | The target temperature for the simulation | measure | 23 |
| 935 | Compressibility | compressibility | The compressibility of the system, used by the barostat | measure | 19 |
| 936 | Reference pressure | ref-p | The target pressure for the simulation | measure | 3 |
| 937 | HETATM record | HETATM | A record in a PDB file for a non-standard atom or small molecule | identifier | 0 |
| 938 | ENDMDL record | ENDMDL | A record in a PDB file that separates multiple models or frames | identifier | 1 |
| 939 | CRYST1 record | CRYST1 | A record in a PDB file that specifies the crystallographic unit cell/simulation box | identifier | 0 |
| 940 | GROMOS96 forcefield | GROMOS96 forcefield | A specific version of the GROMOS force field | model\|data source | 1 |
| 941 | SPC water model file | spc.itp | An include file containing the topology for the SPC water model | data source\|data format | 0 |
| 942 | System directive | [ system ] | A topology directive that defines the name of the system | data format\|identifier | 0 |
| 943 | Molecules directive | [ molecules ] | A topology directive listing the molecules in the system | data format\|identifier | 0 |
| 944 | External Data Representation format | xdr | A standard for portable data used in GROMACS files | data format | 0 |
| 945 | XTC I/O header | xtcio.h | A C++ header file for reading and writing XTC files | data source\|software | 0 |
| 946 | Free energy implementation | Free energy implementation | Methods for calculating free energy differences between states | method\|process | 4 |
| 947 | A state | A state | The initial state in a free energy calculation | state | 1 |
| 948 | B state | B state | The final state in a free energy calculation | state | 3 |
| 949 | Molecule type coupling | couple-moltype | An mdp keyword to select a molecule for free energy coupling | identifier | 0 |

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| 950 | Lambda 0 coupling | couple-lambda0 | An mdp keyword defining non-bonded parameters at lambda=0 | identifier\|state | 0 |
| 951 | Lambda 1 coupling | couple-lambda1 | An mdp keyword defining non-bonded parameters at lambda=1 | identifier\|state | 0 |
| 952 | Intramolecular coupling | couple-intramol | An mdp keyword for intramolecular free energy calculations | identifier | 0 |
| 953 | FEP lambda vector | fep-lambdas | An mdp keyword for the main array of lambda values | identifier\|measure | 0 |
| 954 | Soft-core potential | soft core | A modified potential to prevent singularities in free energy calculations | model | 2 |
| 955 | Coulomb lambda vector | coul-lambdas | An mdp keyword for lambda values for Coulomb interactions | identifier\|measure | 0 |
| 956 | Van der Waals lambda vector | vdw-lambdas | An mdp keyword for lambda values for van der Waals interactions | identifier\|measure | 0 |
| 957 | MBAR analysis script | pymbar script | An external script for analyzing free energy data | software | 0 |
| 958 | dH/d? output file | dhdl.xvg | An output file containing the derivative of the Hamiltonian with respect to lambda | data format | 0 |
| 959 | AWH code | AWH code | A GROMACS module for the Accelerated Weight Histogram method | software\|method | 2 |
| 960 | Free-energy code | free-energy code | The GROMACS module for free energy calculations via lambda coupling | software\|method | 6 |
| 961 | Entropic effects | Entropic effects | Contributions to the PMF from changes in conformational or rotational entropy | model\|measure | 1 |
| 962 | Non-equilibrium pulling | Non-equilibrium pulling | A method to determine free energy differences from non-equilibrium work values | method\|process | 2 |
| 963 | Jarzynski relation | Jarzynski relation | An equality that relates work done during non-equilibrium processes to free energy differences | model | 1 |
| 964 | Collective variable | Collective variables | A function of atomic coordinates used as a reaction coordinate | measure\|model | 5 |
| 965 | Pull group | pull groups | A group of atoms defining a collective variable for pulling | identifier\|chemical entity | 19 |
| 966 | Umbrella pulling | Umbrella pulling | A pull method applying a harmonic potential to a collective variable | method\|model | 5 |
| 967 | Constraint pulling | Constraint pulling | A pull method that constrains the distance of a collective variable | method\|model | 5 |
| 968 | Constant force pulling | Constant force pulling | A pull method that applies a constant force to a collective variable | method\|model | 2 |
| 969 | Flat bottom pulling | Flat bottom pulling | A pull method using a harmonic potential with a zero-force region | method\|model | 1 |
| 970 | External potential pulling | External potential | A pull method where the potential is provided by another module | method\|model | 0 |
| 971 | Pull coordinate geometry | pull-coord?-geometry | An mdp option to set the type of reaction coordinate (distance, angle, etc.) | identifier | 3 |
| 972 | Pull PBC reference COM | pull-pbc-ref-prev-step-com | An mdp option for treating COM of large groups with PBC | identifier | 0 |
| 973 | Pull PBC reference atom | pull-group?-pbcatom | An mdp option to select a reference atom for PBC wrapping | identifier | 0 |
| 974 | Cylinder geometry | cylinder | A pull geometry using only atoms within a cylinder for the reference group | model | 1 |
| 975 | Cylinder radius | pull-cylinder-r | An mdp option for the radius of the cylinder in a cylinder geometry pull | measure | 1 |
| 976 | Cosine weighting | cosine weighting | A weighting profile for atoms in a reference group to handle periodicity | method\|model | 2 |
| 977 | Weighted center of mass | weighted center of mass | A center of mass calculation including additional weighting factors | measure | 1 |
| 978 | Distance geometry | distance | A pull geometry defined by the distance between two groups | model | 0 |
| 979 | Direction geometry | direction | A pull geometry defined by the projection onto a fixed vector | model | 1 |
| 980 | Direction-relative geometry | direction-relative | A pull geometry where the pull vector is defined by two additional groups | model | 0 |
| 981 | Angle geometry | angle | A pull geometry defined by the angle between three groups | model | 0 |
| 982 | Angle-axis geometry | angle-axis | A pull geometry defined by an angle with respect to a fixed axis | model | 0 |
| 983 | Dihedral geometry | dihedral | A pull geometry defined by the dihedral angle between four groups | model | 1 |
| 984 | Transformation pull coordinate | transformation pull coordinate | A meta-coordinate defined by a mathematical expression of other coordinates | model\|measure | 5 |
| 985 | Number of pull groups | pull-ngroups | An mdp option for the total number of pull groups | identifier | 1 |

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| 986 | Number of pull coordinates | pull-ncoords | An mdp option for the number of pull coordinates | identifier | 1 |
| 987 | Pull group name | pull-group?-name | An mdp option to name a pull group | identifier | 0 |
| 988 | Pull coordinate dimension | pull-coord?-dim | An mdp option to specify the dimensions (x,y,z) of the pull force | identifier | 0 |
| 989 | Pull force constant | pull-coord?-k | An mdp option for the force constant of the pull potential | measure | 0 |
| 990 | Pull expression | pull-coord?-expression | An mdp option for the mathematical expression of a transformation coordinate | identifier\|model | 0 |
| 991 | Pull initial value | pull-coord?-init | An mdp option for the initial value of a pull coordinate | measure | 0 |
| 992 | Biasing potential | biasing potential | A history-dependent potential applied to overcome free energy barriers | model | 3 |
| 993 | Wang-Landau algorithm | Wang-Landau | An adaptive Monte Carlo method for calculating the density of states | algorithm\|method | 2 |
| 994 | Local elevation | local elevation | An adaptive biasing method, precursor to metadynamics | algorithm\|method | 2 |
| 995 | Metadynamics | metadynamics | An adaptive biasing method that discourages revisiting configurations by adding Gaussian potentials | algorithm\|method | 6 |
| 996 | Reaction coordinate | ?(x) | The collective variable along which the PMF is calculated | measure\|model | 37 |
| 997 | Umbrella function | Q(?, ?) | The potential function that couples the reaction and reference coordinates | model | 1 |
| 998 | Extended ensemble | extended ensemble | The joint statistical ensemble of system coordinates and a reaction coordinate | model\|state | 5 |
| 999 | Bias function | g(?) | A function of the free energy used to construct the AWH bias | model\|measure | 3 |
| ### | Target distribution | ?(?) | The desired probability distribution along the reference coordinate | model\|state | 40 |
| ### | Free energy update | ?Fn(?) | The correction applied to the free energy estimate at each AWH update | process\|measure | 8 |
| ### | Conditional distribution | ?n(?\|x) | The probability of being at reference coordinate ? given system state x | measure\|model | 2 |
| ### | Reference weight histogram | Wn(?) | A histogram of prior samples that determines the AWH update size | data source\|measure | 2 |
| ### | Convolved bias potential | Un(?) | The effective bias potential applied to the system coordinates | model | 2 |
| ### | Gibbs sampling | Gibbs sampling | A Monte Carlo sampling method used in one mode of AWH | algorithm\|method | 10 |
| ### | Initial stage | initial stage | The first phase of an AWH simulation with exponentially decaying update size | process\|state | 43 |
| ### | Final stage | final stage | The production phase of an AWH simulation with linearly decaying update size | process\|state | 10 |
| ### | Covering | covering | The event of having visited all points along the sampling interval | state\|process | 23 |
| ### | Growth factor | ? | A factor by which the weight histogram is scaled after a covering | measure | 4 |
| ### | Covering criterion | covering criterion | The condition that defines when a sampling interval is covered | method\|model | 1 |
| ### | Peak weight | Wpeak | The target accumulated probability for a point to be considered visited | measure | 0 |
| ### | Initial stage exit criterion | initial stage exit criterion | The heuristic used to transition from the initial to the final stage | method\|model | 1 |
| ### | Uniform target distribution | Pconst(?) | A target distribution that is constant over the sampling interval | model | 0 |
| ### | Cutoff target distribution | Pcut(?) | A target distribution that suppresses sampling in high free energy regions | model | 0 |
| ### | Free energy cutoff | Fcut | The free energy value above which sampling is suppressed in Pcut | measure | 2 |
| ### | Boltzmann target distribution | PBoltz(?) | A target distribution that partially flattens the free energy landscape | model | 0 |
| ### | Local Boltzmann target distribution | PBoltz,loc(?) | A target distribution based on the locally accumulated weight histogram | model | 0 |
| ### | Friction metric | friction metric | A tensor that quantifies the difficulty of sampling along reaction coordinates | measure | 23 |
| ### | AWH metric scaling limit | awh1-target-metric-scaling-limit | An mdp option to limit the scaling of the target distribution by the friction metric | identifier | 0 |
| ### | Walker | walkers | A single simulation in a group of simulations that share a bias potential | process\|identifier | 5 |

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| ### | Covering diameter | Dcover | A parameter for a stricter covering criterion when using multiple walkers | measure | 0 |
| ### | AWH multi-simulation sharing | awh-share-multisim | An mdp option to enable bias sharing between parallel simulations | identifier | 0 |
| ### | AWH share group | awh1-share-group | An mdp option to assign a simulation to a bias sharing group | identifier | 0 |
| ### | Reweighting | Reweighting | A post-processing technique to calculate an unbiased PMF from biased data | method\|process | 7 |
| ### | Diffusion matrix | D(?) | A matrix describing the diffusion on the flattened free energy landscape | measure | 1 |
| ### | Sampling efficiency | ?¹/²(?) | A measure of sampling difficulty derived from the friction metric | measure | 2 |
| ### | Rotation group | rotation group | The group of atoms subjected to enforced rotation | identifier\|chemical entity | 18 |
| ### | Fixed Axis Rotation | Fixed Axis Rotation | A rotation method where the rotation axis is fixed in space | model\|method | 4 |
| ### | Flexible Axis Rotation | Flexible Axis Rotation | A rotation method where the rotation axis can be flexible | model\|method | 5 |
| ### | Isotropic rotation potential | Viso | A harmonic potential that attracts atoms to a rotating reference structure | model | 0 |
| ### | Pivot-Free Isotropic Potential | Viso-pf | A rotation potential where the pivot point is the center of mass | model | 2 |
| ### | Parallel Motion Potential | Vpm | A rotation potential variant that allows free motion along the rotation axis | model | 3 |
| ### | Radial Motion Potential | Vrm | A rotation potential variant that reduces forces restricting radial motion | model | 5 |
| ### | Radial Motion 2 Potential | Vrm2 | A rotation potential that fully eliminates the radial force component | model | 1 |
| ### | Flexible Axis Potential | Vflex | A potential that applies rotation to a set of slabs, allowing for flexibility | model | 2 |
| ### | Soft slabs | soft slabs | A method of defining flexible segments using Gaussian-weighted contributions | model | 1 |
| ### | Translation-tolerant potential | Vflex-t | A flexible axis potential that moves with the center of mass | model | 0 |
| ### | Rotation group index | rot-group? | An mdp parameter to specify the index group for rotation | identifier | 0 |
| ### | Rotation mass weighting | rot-massw | An mdp parameter to enable mass-weighting for rotation | identifier | 0 |
| ### | Rotation Gaussian cutoff | gmin | A cutoff for slab contributions in flexible rotation | measure | 0 |
| ### | Rotation output file | rotation.xvg | An output file for global rotation data | data format | 0 |
| ### | Rotation angles output file | rotangles.xvg | An output file for fitted rotation angles | data format | 0 |
| ### | Rotation slabs output file | rotslabs.xvg | An output file for slab-wise rotation data | data format | 0 |
| ### | Rotation torque output file | rottorque.xvg | An output file for the torque exerted by the rotation potential | data format | 0 |
| ### | Rotation fit method | rot-fit-method | An mdp option to control how the effective rotation angle is determined | identifier | 0 |
| ### | Torque | Torque | The rotational force exerted by the potential | measure | 9 |
| ### | Membrane capacitance | Cmembrane | The capacitance of the membrane, relating charge imbalance to potential difference | measure | 1 |
| ### | Ion swap output file | swapions.xvg | An output file that logs ion exchange events in CompEL | data format | 0 |
| ### | Channel conductance | G | A measure of the rate of ion flow through a channel | measure | 2 |
| ### | Reversal potential | Urev | The transmembrane potential at which the net ion current is zero | measure | 1 |
| ### | Swap frequency | swap-frequency | An mdp option for the frequency of ion swap attempts | identifier | 0 |
| ### | Split group | split-group? | An mdp option defining an index group for a compartment boundary | identifier | 6 |
| ### | Mass-weighted split group | massw-split? | An mdp option to use the center of mass of the split group as the boundary | identifier | 0 |
| ### | Solvent group | solvent-group | An mdp option specifying the group name of solvent molecules | identifier | 1 |
| ### | Number of ion types | iontypes | An mdp option for the number of ion species controlled by CompEL | identifier | 0 |
| ### | Ion type name | iontype?-name | An mdp option for the name of a controlled ion species | identifier | 0 |

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| ### | Ion reference count | iontype?-in-A/B | An mdp option for the target number of ions in a compartment | identifier\|measure | 0 |
| ### | Coupling steps | coupl-steps | An mdp option to time-average ion distributions before swapping | identifier | 1 |
| ### | Swap threshold | threshold | An mdp option for the minimum ion count deviation to trigger a swap | measure | 0 |
| ### | Cylinder definition | cyl?-r/up/down | mdp options to define a virtual cylinder for counting ion permeation | identifier\|measure | 1 |
| ### | CompEL dump variable | GMX_COMPELDUMP | An environment variable to dump the starting structure for CompEL debugging | identifier | 0 |
| ### | Delta lambda | delta-lambda | An mdp option to make the lambda parameter change linearly with time | identifier | 2 |
| ### | Targeted MD | Targeted MD | A simulation method that forces a system from a starting to a target conformation | method | 2 |
| ### | Hydrogen bond-angle vibrations | Hydrogen bond-angle vibrations | High-frequency motions that can be removed to increase the timestep | model | 2 |
| ### | Out-of-plane vibrations | Out-of-plane vibrations | Motions in aromatic rings that can be constrained using virtual sites | model | 1 |
| ### | Cosine acceleration | cosine acceleration | A non-equilibrium method to calculate viscosity by applying a cosine-shaped acceleration profile | method\|algorithm | 6 |
| ### | Shear simulations | Shear simulations | Non-equilibrium simulations that apply a shear flow to the system | method\|process | 2 |
| ### | Deform box | deform | An mdp option to apply a time-dependent deformation to the simulation box | identifier | 0 |
| ### | Tabulated interaction functions | Tabulated interaction functions | A method using pre-calculated look-up tables for potential and force evaluation | method\|model | 3 |
| ### | Cubic spline interpolation | Cubic splines | An algorithm used to interpolate values from the look-up tables | algorithm\|method | 1 |
| ### | User-specified potential | User-specified potential functions | A feature allowing the use of custom potential functions via tables | method\|model | 1 |
| ### | Energy group table | energygrp-table | An mdp option to specify different interaction tables for pairs of energy groups | identifier | 0 |
| ### | Hybrid QM/MM simulation | QM/MM | A simulation method that treats part of a system with quantum mechanics and the rest with molecular mechanics | method\|model | 0 |
| ### | GEEP | GEEP | A Gaussian expansion of the electrostatic potential method for QM/MM coupling | method\|model | 2 |
| ### | Electrostatic embedding | electrostatic embedding | A QM/MM scheme where MM charges are included in the QM Hamiltonian | model | 4 |
| ### | Link atom | link atom | An atom (usually H) used to saturate the valency of a QM atom at the QM/MM boundary | model\|chemical entity | 3 |
| ### | CP2K library | libcp2k | The library version of CP2K that can be linked to other programs | software | 0 |
| ### | QM/MM active | qmmm-cp2k-active | An mdp option to enable the GROMACS-CP2K QM/MM interface | identifier | 0 |
| ### | QM group | qmmm-cp2k-qmgroup | An mdp option to specify the group of atoms to be treated by QM | identifier | 0 |
| ### | QM charge | qmmm-cp2k-qmcharge | An mdp option to specify the total charge of the QM region | identifier\|measure | 0 |
| ### | QM multiplicity | qmmm-cp2k-qmmultiplicity | An mdp option to specify the spin multiplicity of the QM region | identifier\|measure | 0 |
| ### | QM method | qmmm-cp2k-qmmethod | An mdp option to select the QM level of theory in CP2K | identifier | 1 |
| ### | QM input file option | -qmi | A command-line option for grompp to provide a custom CP2K input file | identifier | 0 |
| ### | CPMD | CPMD | The Car-Parrinello Molecular Dynamics software package | software | 33 |
| ### | Additive QM/MM scheme | additive scheme | A QM/MM formulation where the total energy is a sum of QM, MM, and QM/MM terms | model | 0 |
| ### | Link atom pseudo-potential | Link atom pseudo-potential | A specialized pseudo-potential used to cap a dangling bond at the QM/MM boundary | model | 1 |
| ### | Loose coupling | loose coupling | An application coupling model where two programs run as separate processes and communicate | model\|method | 1 |
| ### | MPI client-server | MPI client-server | A communication model used by MiMiC for inter-program data exchange | method\|software | 1 |
| ### | MiMiC integrator | integrator=mimic | An mdp option to enable the MiMiC workflow, delegating integration to the QM code | identifier | 0 |
| ### | MiMiC QM groups | QMMM-grps | An mdp option to specify the QM atoms for the MiMiC interface | identifier | 0 |

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| ### | MiMiC preprocessor script | prepare-qmmm.py | A Python script to assist in generating the CPMD input for MiMiC | software | 0 |
| ### | MiMiC input section | &MIMIC | The section in the CPMD input file containing settings for the MiMiC interface | data format\|identifier | 0 |
| ### | SLURM | SLURM | A workload manager for high-performance computing clusters | software | 5 |
| ### | srun | srun | The SLURM command to launch a parallel job step | software | 5 |
| ### | OpenMPI | OpenMPI | An open-source Message Passing Interface implementation | software | 12 |
| ### | IntelMPI | IntelMPI | Intel's implementation of the Message Passing Interface | software | 2 |
| ### | AMBER DCD format | AMBER DCD-format | A trajectory file format from the AMBER package, readable via VMD plugins | data format | 0 |
| ### | VMD plugin path | VMD_PLUGIN_PATH | An environment variable to specify the location of VMD plugins | identifier | 0 |
| ### | Interactive Molecular Dynamics | IMD | A protocol allowing a running simulation to be controlled and visualized interactively | method\|protocol | 4 |
| ### | NAMD | NAMD | A molecular dynamics program that uses the IMD protocol | software | 3 |
| ### | IMD group | IMD-group | An mdp option to specify the group of atoms for IMD communication | identifier | 1 |
| ### | TCP sockets | TCP sockets | The communication protocol used for IMD between GROMACS and VMD | method\|protocol | 1 |
| ### | IMD port | -imdport | An mdrun switch to specify the TCP port for IMD communication | identifier | 0 |
| ### | IMD wait | -imdwait | An mdrun switch to make the simulation wait for a VMD client connection | identifier | 0 |
| ### | IMD terminate | -imdterm | An mdrun switch to allow terminating the simulation from VMD | identifier | 0 |
| ### | IMD pull | -imdpull | An mdrun switch to allow applying forces from VMD | identifier | 0 |
| ### | Secure Shell forwarding | Secure shell forwarding | A method to securely connect to a remote simulation for IMD | method\|software | 1 |
| ### | Embedding proteins into membranes | Embedding proteins into the membranes | A method to insert a protein into a pre-equilibrated lipid bilayer | method\|process | 0 |
| ### | ProtSqueeze | ProtSqueeze | An early technique for embedding proteins in membranes | method\|algorithm | 2 |
| ### | Forward model | forward model | A model that translates atomic positions into a simulated density | model | 1 |
| ### | Similarity measure | similarity measure | A measure describing the closeness of the simulated and reference densities | measure | 8 |
| ### | Simulated density | ?sim(r) | The density map generated from the atomic coordinates of the simulation | measure\|model | 24 |
| ### | Reference density | ?ref | The target density map, e.g., from cryo-EM, used in density-guided simulations | data source\|measure | 25 |
| ### | Discrete Gauss transform | discrete Gauss transform | The method used to spread atomic densities onto a grid | algorithm\|method | 1 |
| ### | Inner product similarity | Sinner-product | A similarity measure based on the inner product of the two densities | measure | 0 |
| ### | Relative entropy similarity | Srelative-entropy | A similarity measure based on the relative entropy between two densities | measure | 0 |
| ### | Cross-correlation similarity | Scross-correlation | A similarity measure based on the cross-correlation of the two densities | measure | 0 |
| ### | Density-guided simulation force frequency | density-guided-simulation-nst | An mdp option for the frequency of applying density-guided forces | identifier | 0 |
| ### | Density-fitting energy term | Density-fitting | An energy term in the output file representing the density-guided potential | measure | 0 |
| ### | Adaptive force constant scaling | Adaptive force constant scaling | A method to dynamically adjust the force constant in density-guided simulations | method\|algorithm | 1 |
| ### | Reference density map format | mrc format | The file format for the input reference density map | data format | 1 |
| ### | Affine transformations | Affine transformations | Linear transformations (rotation, scaling) applied to coordinates before density calculation | method\|algorithm | 4 |
| ### | Colvars module | Colvars module | A library for calculating and applying biases to collective variables | software\|method | 6 |

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| ### | Colvars configuration file | colvars-configfile | An mdp option specifying the configuration file for Colvars | identifier\|data format | 3 |
| ### | Colvars seed | colvars-seed | An mdp option to set the random seed for Colvars | identifier | 0 |
| ### | Colvars Dashboard | Colvars Dashboard | A VMD extension for preparing and analyzing Colvars simulations | software | 1 |
| ### | Colvars trajectory file | *.colvars.traj | An output file from Colvars containing the time series of collective variables | data format | 0 |
| ### | PLUMED kernel | PLUMED_KERNEL | An environment variable pointing to the PLUMED shared library | identifier | 2 |
| ### | Neural Network Potentials | NNPot | A GROMACS module for using machine learning potentials | method\|model | 4 |
| ### | PyTorch | PyTorch | A machine learning framework used to train models for the NNPot module | software | 9 |
| ### | TorchScript | TorchScript | A way to create serializable and optimizable models from PyTorch code | software | 3 |
| ### | Hybrid NNP/MM Simulations | Hybrid NNP/MM | Simulations combining a neural network potential for a subsystem with a classical force field | method\|model | 2 |
| ### | NNPot active | nnpot-active | An mdp option to enable the neural network potential interface | identifier | 0 |
| ### | NNPot input group | nnpot-input-group | An mdp option defining the group of atoms for the NNP subsystem | identifier | 0 |
| ### | NNPot model inputs | nnpot-model-input[1-4] | mdp options to specify the inputs to the neural network model | identifier | 0 |
| ### | NN device | GMX_NN_DEVICE | An environment variable to specify the device (CPU/GPU) for NNP inference | identifier | 0 |
| ### | TorchANI | TorchANI | A PyTorch-based library for training and using ANI neural network potentials | software | 3 |
| ### | man pages | man pages | Standard UNIX-style online documentation for programs | data source | 17 |
| ### | Analysis | Analysis | The process of extracting scientific insights from simulation data | process | 249 |
| ### | Group concept | group concept | The use of named sets of atoms or molecules in GROMACS analysis | model | 9 |
| ### | Selections | Selections | A flexible syntax for dynamically defining groups of atoms or positions for analysis | method\|software | 144 |
| ### | Default Groups | Default Groups | Pre-defined atom groups available in analysis tools when no index file is provided | identifier\|chemical entity | 7 |
| ### | rlwrap | rlwrap | A utility that provides readline editing capabilities to command-line programs | software | 1 |
| ### | Center-of-mass velocity | center-of-mass velocity | The velocity of the center of mass of the system or a group | measure | 5 |
| ### | Angle dependent RDF | gAB(r, ?) | A radial distribution function that also depends on the angle with respect to an axis | measure | 1 |
| ### | Correlation functions | Correlation functions | Functions that measure the correlation of a property with itself or another property over time | measure\|model | 18 |
| ### | Cross-correlation function | cross-correlation function | A function that measures the correlation between two different properties over time | measure | 1 |
| ### | Correlation time | ?f | The integral of a correlation function, representing a characteristic timescale | measure | 7 |
| ### | Block-averaging | block-averaging | A procedure to estimate statistical error by averaging over blocks of data | method | 1 |
| ### | Fast Fourier Transform | FFT | An algorithm used to efficiently compute correlation functions | algorithm | 3 |
| ### | Rotational autocorrelation | rotational autocorrelation | An autocorrelation function that describes the rotational motion of a vector | measure | 1 |
| ### | Dipole autocorrelation | dipole autocorrelation | An autocorrelation function of the molecular or group dipole moment | measure | 2 |
| ### | Velocity autocorrelation function | velocity autocorrelation function | The autocorrelation function of atomic or molecular velocities | measure | 5 |
| ### | Self diffusion coefficient | DA | A measure of the translational mobility of a particle type | measure | 2 |
| ### | Green-Kubo relation | Green-Kubo relation | A relation that connects transport coefficients to integrals of time correlation functions | model | 1 |
| ### | Dipole correlation time | dipole correlation time | The correlation time of the dipole autocorrelation function | measure | 2 |
| ### | Curve fitting | Curve fitting | The process of finding an analytical function that matches a set of data points | method\|process | 4 |
| ### | Levenberg-Marquardt algorithm | Levenberg-Marquardt algorithm | An algorithm used for non-linear least squares curve fitting | algorithm | 1 |

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| ### | Error estimation function | ?²(t) | A specific function used to estimate errors in time-correlated data | model | 0 |
| ### | Interphase boundary demarcation | Interphase boundary demarcation | The process of identifying the location and width of an interface | process | 1 |
| ### | Density profile fitting function | f(x) | An error function-based model for fitting density profiles across an interface | model | 0 |
| ### | Transverse current autocorrelation function | transverse current autocorrelation function | A correlation function used to compute viscosity | measure | 2 |
| ### | Viscosity from pressure ACF | Viscosity estimation from pressure autocorrelation function | A method to estimate viscosity by fitting the pressure autocorrelation function | method\|model | 0 |
| ### | Biochemical convention | biochemical convention | A definition for dihedral angles where ?=0 is the cis conformation | model | 2 |
| ### | Polymer convention | polymer convention | A definition for dihedral angles where ?=0 is the trans conformation | model | 4 |
| ### | Root mean square deviation | RMSD | A measure of the average distance between the atoms of superimposed structures | measure | 5 |
| ### | Covariance analysis | Covariance analysis | A method to identify correlated motions in a system, also known as PCA | method\|process | 14 |
| ### | Principal component analysis | principal component analysis | A statistical method to find the principal modes of variation in a dataset | method\|algorithm | 7 |
| ### | Essential dynamics | essential dynamics | An application of principal component analysis to molecular dynamics trajectories | method\|process | 14 |
| ### | Covariance matrix | C | A matrix whose elements are the covariances between atomic coordinate fluctuations | measure\|model | 16 |
| ### | Eigenvectors | eigenvectors | The principal modes of motion obtained from diagonalizing the covariance matrix | measure\|model | 72 |
| ### | Eigenvalues | eigenvalue ?i | The mean square fluctuation along the corresponding principal mode | measure | 23 |
| ### | Subspace overlap | subspace overlap | A measure of the similarity between two subspaces spanned by eigenvectors | measure | 2 |
| ### | Cosine content | cosine content | A measure to check if principal components correspond to random diffusion | measure | 6 |
| ### | Dihedral principal component analysis | Dihedral principal component analysis | Principal component analysis performed on dihedral angles | method\|process | 2 |
| ### | Hydrogen bonds | Hydrogen bonds | A non-covalent interaction involving a hydrogen atom and an electronegative atom | model\|chemical entity | 53 |
| ### | Hydrogen bond existence map | H-bond existence map | A 2D plot showing the existence of H-bonds over time | data format | 0 |
| ### | Protein-related items | Protein-related items | Analysis specific to protein structure and dynamics | process | 2 |
| ### | Interface-related items | Interface-related items | Analysis specific to systems with interfaces, like membranes | process | 2 |
| ### | Order parameter | Sz | A measure of the orientational order of molecular axes with respect to a reference axis | measure | 16 |
| ### | Single Sum Virial | Single Sum Virial | An efficient method for calculating the virial in GROMACS | method\|algorithm | 3 |
| ### | Shift vector | ?i | A vector used in periodic systems to find the nearest image of an atom | model | 7 |
| ### | Intra-molecular shift | mol-shift | A method to handle periodicity for bonded interactions within a molecule | method\|algorithm | 1 |
| ### | Virial from SHAKE | Virial from SHAKE | The contribution to the virial from the SHAKE constraint forces | measure | 1 |
| ### | Inner Loops for Water | Inner Loops for Water | Specially optimized code loops for calculating water interactions in GROMACS | software\|algorithm | 1 |
| ### | Formulae for averaging | Formulae for averaging | Equations used for calculating averages and fluctuations from trajectory data | model | 2 |
| ### | Partial sum | Xn,m | A sum of a quantity over a part of a data series, used in sequential averaging algorithms | measure | 2 |
| ### | Partial variance | ?²n,m | The variance of a quantity over a part of a data series | measure | 2 |
| ### | pydoc | pydoc | A Python tool to generate documentation from Python modules | software | 4 |
| ### | pip | pip | The standard package installer for Python | software | 83 |
| ### | virtual environment | virtual environment | An isolated Python environment that allows for managing separate package installations | software | 19 |
| ### | mpi4py | mpi4py | A Python package providing bindings for the Message Passing Interface (MPI) | software | 36 |

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|---|---|---|---|---|---|
| ### | ensurepip | ensurepip | A Python module to ensure that the pip installer is available | software | 2 |
| ### | setuptools | setuptools | A Python package that provides tools for packaging Python projects | software | 7 |
| ### | pytest | pytest | A framework for writing and running tests for Python code | software | 2 |
| ### | MPI launcher | mpiexec, mpirun | A command used to launch parallel applications using MPI | software | 3 |
| ### | MPI compiler wrapper | mpicc | A compiler wrapper for compiling C code with MPI libraries | software | 4 |
| ### | Offline install | Offline install | The process of installing a package without an internet connection | process | 2 |
| ### | CMAKE_INSTALL_PREFIX | CMAKE_INSTALL_PREFIX | A CMake variable that specifies the installation directory for a project | identifier | 9 |
| ### | venv | venv | A Python module for creating lightweight virtual environments | software | 11 |
| ### | Conda | Conda | A package, dependency and environment management system | software | 4 |
| ### | system-site-packages | --system-site-packages | An option for venv to include system-level packages in the virtual environment | identifier | 3 |
| ### | pybind11 | pybind11 | A lightweight header-only library for creating Python bindings of C++ code | software | 10 |
| ### | wheel package | wheel | A built-distribution format for Python packages | data format | 0 |
| ### | pyproject.toml | pyproject.toml | A file used to specify build system requirements for Python projects | data format | 3 |
| ### | scikit-build-core | scikit-build-core | A build backend for Python packages with C++/CMake components | software | 2 |
| ### | gmxapi_ROOT | gmxapi_ROOT | An environment variable to hint at the GROMACS installation location for gmxapi | identifier | 9 |
| ### | gromacs-hints.cmake | gromacs-hints.cmake | A CMake cache file providing hints about the GROMACS build configuration | data format | 3 |
| ### | python -m build | python -m build | A command to build a Python package from source | software | 2 |
| ### | sdist | sdist | A source distribution format for Python packages | data format | 2 |
| ### | twine | twine | A utility for publishing Python packages to the Python Package Index (PyPI) | software | 2 |
| ### | ImportError | ImportError | A Python exception raised when a module cannot be imported | state | 4 |
| ### | enum34 | enum34 | An older backported enumeration package for Python that can cause conflicts | software | 2 |
| ### | ModuleNotFoundError | ModuleNotFoundError | A Python exception raised when a required module is not found | state | 1 |
| ### | gmxapi support library | gmxapi support library | The C++ library component of gmxapi that must be found during installation | software | 1 |
| ### | git pull --rebase | git pull --rebase | A git command to update a local branch, replaying local commits on top of the fetched branch | software | 3 |
| ### | gmxapi.exceptions.Error | gmxapi.exceptions.Error | The base exception class for the gmxapi package | software | 3 |
| ### | Logging facility | Logging | The Python module used by gmxapi for status messages and logging | software | 0 |
| ### | mpiexec | mpiexec | A command to launch MPI parallel jobs | software | 10 |
| ### | mpi_bindings | mpi_bindings | A gmxapi feature indicating that it was built with MPI support | identifier | 3 |
| ### | result() | result() | A method on a gmxapi data object to trigger execution and retrieve the output | software | 15 |
| ### | ensemble operation | ensemble operation | A gmxapi operation that is applied to a list of inputs, producing a list of outputs | process | 4 |
| ### | input_files | input_files | A parameter for commandline_operation to specify input file dependencies | identifier | 9 |
| ### | output_files | output_files | A parameter for commandline_operation to specify output files | identifier | 11 |
| ### | returncode | returncode | An output of a commandline_operation representing the process exit code | measure | 3 |
| ### | stderr | stderr | An output of a commandline_operation representing the standard error stream | data source | 22 |
| ### | stdout | stdout | An output of a commandline_operation representing the standard output stream | data source | 13 |
| ### | function_wrapper | gmxapi.function_wrapper | A decorator to convert a Python function into a gmxapi-compatible operation | software | 8 |

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| ### | work graph | work graph | A directed acyclic graph of operations and data dependencies managed by gmxapi | model | 4 |
| ### | Future | Future | A gmxapi object representing a data value that will be available in the future | software | 56 |
| ### | while loop | gmxapi.while_loop | A gmxapi operation to execute another operation repeatedly until a condition is met | software | 2 |
| ### | OperationReference | gmxapi.abc.OperationReference | The client interface to a configured computational operation in the work graph | software | 2 |
| ### | OutputDataProxy | OutputDataProxy | A proxy object providing access to the named outputs of an operation | software | 9 |
| ### | run() | run() | A method on an operation reference to explicitly assert its execution | software | 8 |
| ### | commandline_operation | commandline_operation | A gmxapi function to wrap command-line tools | software | 19 |
| ### | config | gmxapi.utility.config | A gmxapi utility function to get the detected GROMACS configuration | software | 52 |
| ### | join_path | gmxapi.utility.join_path | A gmxapi utility to create a future path object for data flow | software | 2 |
| ### | concatenate_lists | gmxapi.concatenate_lists | A gmxapi helper to combine multiple lists into a single data flow object | software | 1 |
| ### | join_arrays | gmxapi.join_arrays | A gmxapi helper to concatenate two array-like data sources | software | 1 |
| ### | logical_not | gmxapi.logical_not | A gmxapi operation for boolean negation | software | 2 |
| ### | make_constant | gmxapi.make_constant | A gmxapi operation to provide a predetermined value at runtime | software | 1 |
| ### | filtered_mpi_environ | gmxapi.runtime.filtered_mpi_environ | A gmxapi utility to get a copy of the environment with MPI variables removed | software | 6 |
| ### | filtered_prefixes | gmxapi.runtime.filtered_prefixes | A tuple of MPI-related environment variable prefixes filtered by default | data source | 2 |
| ### | ApiError | gmxapi.exceptions.ApiError | An exception for an API operation attempted with an incompatible object | state | 1 |
| ### | DataShapeError | gmxapi.exceptions.DataShapeError | An exception for an object having an incompatible shape | state | 1 |
| ### | FeatureNotAvailableError | gmxapi.exceptions.FeatureNotAvailableError | An exception for a requested feature not being available in the environment | state | 3 |
| ### | MissingImplementationError | gmxapi.exceptions.MissingImplementationError | An exception indicating a feature is specified but not implemented | state | 2 |
| ### | ProtocolError | gmxapi.exceptions.ProtocolError | An exception for unexpected API behavior or protocol violation | state | 2 |
| ### | TypeError | gmxapi.exceptions.TypeError | An exception for an incompatible data type | state | 1 |
| ### | UsageError | gmxapi.exceptions.UsageError | An exception for unsupported syntax or call signatures | state | 2 |
| ### | ValueError | gmxapi.exceptions.ValueError | An exception for a user-provided value that cannot be interpreted | state | 1 |
| ### | Warning | gmxapi.exceptions.Warning | The base warning class for gmxapi exceptions | state | 84 |
| ### | gmx.version module | gmx.version | A gmxapi module for version and release information | software | 2 |
| ### | api_is_at_least | gmxapi.version.api_is_at_least | A function to check if the installed gmxapi supports a requested API level | software | 3 |
| ### | has_feature | gmxapi.version.has_feature | A function to query whether a named feature is available in the installation | software | 7 |
| ### | Core API | Core API | The C++ extension module providing Python access to the GROMACS C++ API | software | 2 |
| ### | from_tpr | gmxapi._gmxapi.from_tpr | A Core API function to initialize a system container from a TPR file | software | 2 |
| ### | create_context | gmxapi._gmxapi.create_context | A Core API function to manage resources and the software environment | software | 5 |
| ### | copy_tprfile | gmxapi._gmxapi.copy_tprfile | A Core API function to copy a TPR file | software | 1 |
| ### | read_tprfile | gmxapi._gmxapi.read_tprfile | A Core API function to get a handle to a TPR file resource | software | 1 |
| ### | write_tprfile | gmxapi._gmxapi.write_tprfile | A Core API function to write a new TPR file | software | 1 |
| ### | rewrite_tprfile | gmxapi._gmxapi.rewrite_tprfile | A Core API function to copy and modify a TPR file | software | 1 |
| ### | Context | gmxapi._gmxapi.Context | A Core API class for managing simulation context and plugins | software | 47 |

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| ### | MDArgs | gmxapi._gmxapi.MDArgs | A Core API class for managing mdrun runtime parameters | software | 5 |
| ### | MDSession | gmxapi._gmxapi.MDSession | A Core API class representing a running simulation session | software | 4 |
| ### | MDSystem | gmxapi._gmxapi.MDSystem | A Core API class representing a system to be simulated | software | 3 |
| ### | SimulationParameters | gmxapi._gmxapi.SimulationParameters | A Core API class for accessing and modifying simulation parameters | software | 7 |
| ### | TprFile | gmxapi._gmxapi.TprFile | A Core API class representing a TPR file resource | software | 5 |
| ### | (Non-)Bonded Library (NB-LIB) API | NB-LIB API | A GROMACS library for programmatically defining molecular simulations | software | 6 |
| ### | nblib | nblib | The C++ namespace for the Non-Bonded Library | identifier | 18 |
| ### | ParticleName | ParticleName | A data structure for the name of a particle type | data format | 14 |
| ### | Mass | Mass | A data structure for the mass of a particle type | data format | 324 |
| ### | RVec | gmx::RVec | A data type for holding 3D vector quantities | data format | 10 |
| ### | ParticleType | ParticleType | A class to define the properties of a particle type in NB-LIB | software | 9 |
| ### | ParticleTypeInteractions | ParticleTypeInteractions | A class to define non-bonded interactions between particle types | software | 4 |
| ### | Molecule | Molecule | A class to define a molecule from its constituent particles and interactions | software | 256 |
| ### | HarmonicBondType | HarmonicBondType | A class for defining a harmonic bond interaction | software | 2 |
| ### | DefaultAngle | DefaultAngle | A class for defining a default angle interaction | software | 2 |
| ### | Box | Box | A class to define the simulation box dimensions | software | 410 |
| ### | NBKernelOptions | NBKernelOptions | A class to configure options for non-bonded interaction kernels | software | 3 |
| ### | TopologyBuilder | TopologyBuilder | A class to construct the system topology from molecules and interactions | software | 7 |
| ### | SimulationState | SimulationState | An object representing a snapshot of the system state | software | 7 |
| ### | ForceCalculator | ForceCalculator | A class to compute forces on all particles in the system | software | 5 |
| ### | LeapFrog | LeapFrog | An integrator that uses the leap-frog algorithm | algorithm\|software | 2 |
| ### | Developer Guide | Developer Guide | Documentation for developers contributing to GROMACS | data source | 11 |
| ### | Checklist | Checklist | A list of points to check before submitting code for review | process | 5 |
| ### | Preparing code for submission | Preparing code for submission | Guidelines for how to prepare and submit changes to GROMACS | process | 2 |
| ### | Codebase overview | Codebase overview | A high-level description of the GROMACS source code organization | data source | 6 |
| ### | Source code organization | Source code organization | Details on the structure and dependencies of the GROMACS source code | data source | 5 |
| ### | libgromacs | libgromacs | The main GROMACS library containing the core simulation engine | software | 37 |
| ### | testutils | testutils | A library of shared utility code for writing tests | software | 9 |
| ### | Google Test | Google Test | A C++ testing framework used by GROMACS | software | 11 |
| ### | legacy_modules | legacy_modules | A CMake target for older GROMACS interfaces | software | 3 |
| ### | Documentation organization | Documentation organization | The structure of the GROMACS documentation source files | data source | 5 |
| ### | Doxygen documentation | Doxygen documentation | The API documentation for the C++ code, generated by Doxygen | data source | 20 |
| ### | Build system overview | Build system overview | An overview of the CMake-based build system for GROMACS | data source | 14 |
| ### | Build types | Build types | Predefined CMake configurations for building GROMACS (e.g., Release, Debug) | identifier | 8 |
| ### | RelWithDebInfo | RelWithDebInfo | A build type with optimizations and debugging symbols | identifier | 1 |
| ### | TSAN | ThreadSanitizer | A sanitizer build to detect data races in multi-threaded code | software | 6 |

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| ### | ASAN | AddressSanitizer | A sanitizer build to detect memory errors | software | 2 |
| ### | MSAN | MemorySanitizer | A sanitizer build to detect reads of uninitialized memory | software | 1 |
| ### | UBSAN | UndefinedBehaviorSanitizer | A sanitizer build to detect undefined behavior during execution | software | 1 |
| ### | Compiler flags | Compiler flags | Options passed to the compiler to control the build process | identifier | 12 |
| ### | GMX_SKIP_DEFAULT_CFLAGS | GMX_SKIP_DEFAULT_CFLAGS | A CMake variable to skip automatic addition of default compiler flags | identifier | 2 |
| ### | GMX_BUILD_OWN_FFTW | GMX_BUILD_OWN_FFTW | A CMake variable to build the FFTW library from source | identifier | 2 |
| ### | GMX_BUILD_SHARED_EXE | GMX_BUILD_SHARED_EXE | A CMake variable to build executables as shared binaries | identifier | 2 |
| ### | GMX_COMPILER_WARNINGS | GMX_COMPILER_WARNINGS | A CMake variable to enable a strict set of compiler warnings | identifier | 1 |
| ### | GMX_ENABLE_CCACHE | GMX_ENABLE_CCACHE | A CMake variable to enable the use of the ccache compiler wrapper | identifier | 2 |
| ### | GMX_DOUBLE | GMX_DOUBLE | A CMake variable to build GROMACS in double precision | identifier | 5 |
| ### | GMX_EXTERNAL_TNG | GMX_EXTERNAL_TNG | A CMake variable to use an external TNG library | identifier | 2 |
| ### | GMX_FFT_LIBRARY | GMX_FFT_LIBRARY | A CMake variable to choose the CPU FFT library | identifier | 1 |
| ### | GMX_GPU | GMX_GPU | A CMake variable to choose the backend for GPU offload | identifier | 4 |
| ### | GMX_OPENMP | GMX_OPENMP | A CMake variable to enable OpenMP support | identifier | 2 |
| ### | GMX_SIMD | GMX_SIMD | A CMake variable to choose the SIMD instruction set | identifier | 13 |
| ### | GMX_THREAD_MPI | GMX_THREAD_MPI | A CMake variable to enable thread-MPI support | identifier | 2 |
| ### | GMX_USE_PLUGINS | GMX_USE_PLUGINS | A CMake variable to enable support for dynamic plugins | identifier | 2 |
| ### | GMX_USE_TNG | GMX_USE_TNG | A CMake variable to use the TNG library for trajectory I/O | identifier | 3 |
| ### | GMX_VMD_PLUGIN_PATH | GMX_VMD_PLUGIN_PATH | A CMake variable to specify the path to VMD plugins | identifier | 1 |
| ### | BUILD_TESTING | BUILD_TESTING | A standard CTest variable to enable or disable tests | identifier | 3 |
| ### | GMX_DEVELOPER_BUILD | GMX_DEVELOPER_BUILD | A CMake variable to enable developer-specific build features | identifier | 3 |
| ### | GMX_CLANG_TIDY | GMX_CLANG_TIDY | A CMake variable to enable static analysis with clang-tidy | identifier | 1 |
| ### | GMX_INSTALL_LEGACY_API | GMX_INSTALL_LEGACY_API | A CMake variable to install legacy C++ headers | identifier | 3 |
| ### | GMX_BUILD_MANUAL | GMX_BUILD_MANUAL | A CMake variable to enable building the PDF reference manual | identifier | 3 |
| ### | GMX_BUILD_UNITTESTS | GMX_BUILD_UNITTESTS | A CMake variable to build the unit test binaries | identifier | 3 |
| ### | REGRESSIONTEST_DOWNLOAD | REGRESSIONTEST_DOWNLOAD | A CMake variable to download the regression test suite | identifier | 1 |
| ### | REGRESSIONTEST_PATH | REGRESSIONTEST_PATH | A CMake variable specifying the path to the regression test suite | identifier | 3 |
| ### | Suppressing issues | Suppressing issues | A mechanism to filter out known issues from the checker script reports | process | 1 |
| ### | suppressions.txt | suppressions.txt | The file containing the list of suppressed issues for the source checker | data format | 2 |
| ### | Include dependency graphs | Include dependency graphs | Visual representations of #include dependencies between modules or files | data format | 3 |
| ### | dot | dot | A graph visualization software from the graphviz package | software | 9 |
| ### | Automatic source code formatting | Automatic source code formatting | The process of automatically applying code style guidelines | process | 5 |
| ### | Black | Black | An opinionated Python code formatter | software | 21 |
| ### | clang-tidy | clang-tidy | A clang-based C++ linter tool for static analysis | software | 41 |
| ### | copyright.py | copyright.py | A script for checking and updating copyright headers in source files | software | 3 |

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| ### | copyright.sh | copyright.sh | A shell script that runs copyright.py on modified files | software | 6 |
| ### | clang-format.sh | clang-format.sh | A shell script that runs clang-format on modified files | software | 8 |
| ### | clang-tidy.sh | clang-tidy.sh | A shell script that runs clang-tidy on modified files | software | 8 |
| ### | git filters | git filters | A git mechanism to automatically process files on checkout or check-in | software | 4 |
| ### | git pre-commit hook | git pre-commit hook | A script that is run automatically by git before a commit is created | software | 1 |
| ### | reformat_all.sh | reformat_all.sh | A script to apply formatting to all applicable files in the source tree | software | 2 |
| ### | git blame | git blame | A git command to show what revision and author last modified each line of a file | software | 3 |
| ### | .git-blame-ignore-revs | .git-blame-ignore-revs | A file listing commits to be ignored by git blame, typically for formatting changes | data format | 2 |
| ### | Unit testing | Unit testing | The practice of testing individual components or modules of a software | process | 10 |
| ### | CTest | CTest | The testing tool that comes with CMake, used to automate test execution | software | 16 |
| ### | gmx_add_unit_test() | gmx_add_unit_test() | A CMake macro for declaring a GROMACS unit test binary | software | 1 |
| ### | Physical validation | Physical validation | Tests that check whether simulation results correspond to physical or mathematical expectations | process | 11 |
| ### | Integrator convergence | Integrator convergence | A physical validation test checking the conservation properties of an integrator | process | 2 |
| ### | Kinetic energy distribution | Kinetic energy distribution | A physical validation test checking if the KE follows a Maxwell-Boltzmann distribution | process | 3 |
| ### | Distribution of configurational quantities | Distribution of configurational quantities | A physical validation test comparing distributions between different state points | process | 2 |
| ### | Ensemble tests | Ensemble tests | Physical validation tests performed on generated statistical ensembles | process | 1 |
| ### | Known issues relevant for developers | Known issues relevant for developers | A list of known, unsolved issues that may be of interest to developers | data source | 4 |
| ### | GPU timer with OpenCL | Issues with GPU timer with OpenCL | A known issue regarding GPU timer corruption in OpenCL debug builds | state | 2 |
| ### | GPU emulation | GPU emulation | A mode for running GPU code on a CPU, which has known issues | software | 4 |
| ### | PME decomposition automated task assignment | PME decomposition automated task assignment | A feature for automatically assigning tasks in PME simulations that has known issues | software | 2 |
| ### | Public C++ API | Public C++ API | The set of C++ interfaces intended for use by external client software | software | 6 |
| ### | Client build system support | Client build system support | Mechanisms provided by GROMACS to help configure the build system of client software | software | 2 |
| ### | Compiler toolchain | Compiler toolchain | The set of compilers and linkers used to build the software | software | 2 |
| ### | gmxapi CMake package | gmxapi CMake package | The CMake configuration files that support find_package(gmxapi) | software | 2 |
| ### | Imported target | Imported target | A CMake target that represents a pre-existing dependency | software | 1 |
| ### | gromacs (and gromacs$GROMACS_SUFFIX packages) | gromacs package | The CMake configuration files that support find_package(GROMACS) | software | 2 |
| ### | Release Notes | Release Notes | Documentation recording changes made in GROMACS releases | data source | 163 |
| ### | MTTK pressure coupling | MTTK pressure coupling | A barostat method that has been deprecated | method\|algorithm | 1 |
| ### | HDF5-based H5MD format | H5MD | A hierarchical data format for storing molecular dynamics data | data format | 0 |
| ### | AMD HIP | AMD HIP | A C++ runtime API and kernel language for GPU computing on AMD devices | software | 7 |
| ### | oneMath | oneMath | An interface library for GPU FFTs, part of oneAPI | software | 8 |
| ### | rocFFT | rocFFT | AMD's library for Fast Fourier Transforms on ROCm-enabled GPUs | software | 8 |
| ### | NVSHMEM | NVSHMEM | A parallel programming model from NVIDIA for GPU memory communication | software | 26 |

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| ### | Pymbar | Pymbar | A Python library for MBAR analysis, for which compatibility has been updated | software | 4 |
| ### | FetchContent | FetchContent | A CMake module for acquiring dependencies at configure time | software | 2 |
| ### | cgroups | cgroups | A Linux kernel feature for resource management, used for CPU limit detection | software | 3 |
| ### | NBNxM | NBNxM | A non-bonded kernel implementation in GROMACS | software | 7 |
| ### | mass-repartition-factor | mass-repartition-factor | An mdp option for flexible hydrogen mass repartitioning | identifier | 3 |
| ### | virtual_sites1 | virtual_sites1 | A virtual site constructed from a single atom | model | 2 |
| ### | nstpcouple | nstpcouple | An mdp option for the frequency of pressure coupling | identifier | 11 |
| ### | GMX_VERLET_BUFFER_PRESSURE_TOLERANCE | GMX_VERLET_BUFFER_PRESSURE_TOLERANCE | An environment variable to control the pressure deviation tolerance from missing LJ interactions | identifier | 2 |
| ### | GMX_ENABLE_DIRECT_GPU_COMM | GMX_ENABLE_DIRECT_GPU_COMM | An environment variable to enable direct GPU communication for halo exchange | identifier | 6 |
| ### | VSITE2FD | VSITE2FD | A virtual site type constructed from two atoms with a fixed distance | model | 2 |
| ### | pi-helices | Pi-helices | A type of protein secondary structure | chemical entity | 2 |
| ### | editconf -noc | gmx editconf -noc | An option to prevent centering the system in the box | identifier | 1 |
| ### | libc++ | libc++ | The C++ standard library implementation used by Clang | software | 6 |
| ### | CUDA Graphs | CUDA Graphs | A feature in CUDA to define and launch a sequence of GPU operations as a single unit | software | 10 |
| ### | constr_vsiten | constr_vsiten | A function for constraining virtual sites constructed from N atoms | software | 2 |
| ### | LJ-14 parameters | LJ-14 parameters | Non-bonded parameters specifically for 1-4 interactions | measure | 1 |
| ### | state_prev.cpt | state_prev.cpt | The backup checkpoint file from the previous step | data format | 2 |
| ### | CMake config package | CMake config package | Files generated by CMake that allow other projects to find and use a library | data format | 1 |
| ### | hipSYCL | hipSYCL | An open-source SYCL implementation that can target AMD and NVIDIA GPUs | software | 11 |
| ### | gmxapi.runtime.filtered_mpi_environ() | gmxapi.runtime.filtered_mpi_environ() | A gmxapi utility to provide an MPI-free environment for subprocesses | software | 6 |
| ### | gmxapi.simulation.workflow.from_tpr() | gmxapi.simulation.workflow.from_tpr() | A gmxapi function to create a workflow from a TPR file | software | 1 |
| ### | convert-tpr | gmx convert-tpr | A GROMACS tool for modifying binary run input files | software | 32 |
| ### | PME pipelining | PME pipelining | A technique to overlap computation and communication in the PME algorithm | method\|algorithm | 4 |
| ### | cuFFTMp | cuFFTMp | A multi-process, multi-GPU FFT library from NVIDIA | software | 15 |
| ### | NbnxmSetupTest.CanCreateNbnxmGPU | NbnxmSetupTest.CanCreateNbnxmGPU | A specific unit test for the NBNxM kernel setup | software | 2 |
| ### | RISC-V | RISC-V | An open standard instruction set architecture | software | 6 |
| ### | Apple silicon GPUs | Apple silicon GPUs | GPUs designed by Apple, supported via the OpenCL backend | software | 1 |
| ### | clFFT | clFFT | An OpenCL FFT library | software | 19 |
| ### | AWH friction metric | AWH friction metric | A measure of sampling difficulty in AWH, which is now shared between walkers | measure | 8 |
| ### | grompp -maxwarn | grompp -maxwarn | An option to set the maximum number of warnings before grompp aborts | identifier | 2 |
| ### | CUDA PME spread | CUDA PME spread | The part of the PME calculation that spreads charges to the grid, running on CUDA | software | 1 |
| ### | Gapsys soft-core function | Gapsys soft-core function | A specific soft-core potential formulation for free energy calculations | model | 1 |
| ### | mdrun -rerun | mdrun -rerun | An mdrun option to re-calculate energies and forces for a given trajectory | identifier | 13 |
| ### | muParser | muParser | A mathematical expression parser library used in GROMACS | software | 10 |

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| ### | AMD RDNA | AMD RDNA | An AMD GPU architecture | software | 2 |
| ### | nvcc | nvcc | The NVIDIA CUDA compiler | software | 20 |
| ### | AVX_128_FMA SIMD | AVX_128_FMA | A specific SIMD instruction set with FMA4 support | software | 1 |
| ### | PME coordinate padding | PME coordinate padding | A buffer region in memory for PME calculations | data format | 1 |
| ### | tinyXML-2 | tinyXML-2 | A small, efficient C++ XML parser library | software | 3 |
| ### | master branch | master branch | The former name of the main development branch in git | identifier | 3 |
| ### | main branch | main branch | The current name of the main development branch in git | identifier | 6 |
| ### | rtpi | rtpi | The radius of the test particle for insertion | measure | 4 |
| ### | gmx sans | gmx sans | A tool for calculating Small-Angle Neutron Scattering profiles | software | 14 |
| ### | gmx order -unsat | gmx order -unsat | A removed option from gmx order | identifier | 0 |
| ### | dVremain/dl | dVremain/dl | The remaining part of the free energy derivative after analytical contributions are subtracted | measure | 2 |
| ### | nstdhdl | nstdhdl | The frequency for writing dH/dL data to the output file | identifier | 13 |
| ### | Me2PO4 | Me2PO4 | Dimethylphosphate, a molecule for which OPLS-AA torsion parameters were corrected | chemical entity | 2 |
| ### | GROMOS force field | GROMOS force field | A family of force fields, for which disulfide bridge generation was fixed | model\|data source | 3 |
| ### | Core spin-up code | Core spin-up code | Code to wake up CPU cores on non-x86 platforms, which has been removed | software | 1 |
| ### | gmxapi.mdrun runtime_args | runtime_args | A new keyword argument to pass arbitrary runtime arguments to gmxapi.mdrun | identifier | 0 |
| ### | LJ PME | LJ PME | A known issue with LJ PME and free energy calculations was fixed | method\|algorithm | 9 |
| ### | gmxapi MD plugin binding | gmxapi MD plugin binding | A fix for handling MD extension code in gmxapi | software | 1 |
| ### | NB-LIB | NB-LIB | A new non-bonded interaction API | software | 17 |
| ### | ARM SVE | ARM SVE | A SIMD instruction set for ARM processors | software | 5 |
| ### | Fujitsu A64FX | Fujitsu A64FX | A CPU with ARM SVE support | software | 3 |
| ### | density-guided-simulation-normalize-densities | density-guided-simulation-normalize-densities | An mdp option for which the normalization behavior was changed | identifier | 3 |
| ### | gmxapi Python package | gmxapi Python package | A bug causing unnecessary MPI initialization on import was fixed | software | 23 |
| ### | Xeon Phi support | The Xeon Phi support will be removed | Support for this Intel accelerator is deprecated and will be removed | software | 2 |
| ### | AWH cover diameter | AWH cover diameter | A parameter for AWH which now has units of degrees for angles | measure | 2 |
| ### | GPU LINCS | GPU LINCS | A bug with missing synchronization in the CUDA implementation of LINCS was fixed | algorithm\|software | 3 |
| ### | g_bar | g_bar | An old tool name for which references were fixed | software | 1 |
| ### | pullf.xvg | pullf.xvg | A pull code output file that is now correctly written during a rerun | data format | 6 |
| ### | GROMOS force fields | GROMOS force fields | A fix for an incorrect bond type for C and +N in the ACE capping group | model\|data source | 12 |
| ### | Hygon Dhyana CPU | Hygon Dhyana CPU | A CPU architecture for which hardware detection and heuristics have been added | software | 1 |
| ### | CODATA 2018 | CODATA 2018 | A set of fundamental physical constants to which GROMACS has been updated | data source | 1 |
| ### | PDB CONECT record | PDB CONECT record | A record in PDB files for which duplicate output was fixed | data format | 1 |
| ### | gmxapi MPI awareness | Improved MPI awareness and task uniqueness for gmxapi Python runner | Changes to make gmxapi operations aware of the MPI environment and execute in unique directories | software | 0 |
| ### | demux.pl | demux.pl | A script for post-processing replica exchange trajectories, for which a discontinuity issue was fixed | software | 1 |

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| ### | pull-geometry 'direction' | pull-geometry 'direction' | A fix to allow this pull coordinate geometry to be periodic with AWH | identifier | 0 |
| ### | pull geometry direction-periodic | pull geometry direction-periodic | A pull geometry that was disallowed with AWH due to potential incorrect behavior | identifier | 2 |
| ### | gmx cluster -clndx | gmx cluster -clndx | An option for which the reported trajectory frame indices were corrected | software | 2 |
| ### | gmx editconf -f in.pdb -o out.pdb | gmx editconf -f in.pdb -o out.pdb | A command that now correctly preserves chain IDs | software | 1 |
| ### | gmx mdrun -membed | gmx mdrun -membed | A deprecated feature for embedding a protein in a membrane | software | 4 |
| ### | gmx mdrun -rerun | gmx mdrun -rerun | A deprecated feature for re-calculating energies from a trajectory | software | 3 |
| ### | Integrator .mdp options | Integrator .mdp options will only contain dynamical integrators | A change to separate dynamical integrators from energy minimization and normal-mode analysis | software | 3 |
| ### | Intel KNC (MIC) support | Intel KNC (MIC) support | A deprecated architecture | software | 1 |
| ### | Sparc64 HPC ACE | Sparc64 HPC ACE | A deprecated architecture | software | 2 |
| ### | Legacy SIMD architecture support | Legacy SIMD architecture support | Older SIMD implementations that are deprecated | software | 1 |
| ### | Constant-acceleration MD | Constant-acceleration MD | A feature that has been broken for many years and will be removed | software | 1 |
| ### | Reading .pdo files in gmx wham | Reading .pdo files in gmx wham | A removed capability to read an old output format | software | 1 |
| ### | 32bit architectures | Support for 32bit architectures | A deprecated feature due to lack of large-scale resources for testing | software | 4 |
| ### | Free-energy soft-core power 48 | Free-energy soft-core power 48 | A rarely used and therefore deprecated soft-core power | software | 4 |
| ### | Armv7 support | Support for Armv7 | A deprecated architecture due to lack of resources for support and fixes | software | 0 |
| ### | Generation of virtual sites for aromatic rings | Generation of virtual sites to replace aromatic rings in standard residues | A deprecated feature thought to produce artifacts and in need of simplification | software | 0 |
| ### | Benchmarking options | Benchmarking options only available with gmx benchmark | Options like -confout moved from mdrun to a dedicated benchmark tool | software | 7 |
| ### | gmx mdrun -nsteps | gmx mdrun -nsteps | A deprecated option whose convenience was outweighed by its poor implementation | software | 8 |
| ### | Group cut-off scheme | Group cut-off scheme | A removed feature that several kinds of simulations depended on | software | 5 |
| ### | Hygon Dhyana CPU architecture | Added support for Hygon Dhyana CPU architecture | Support for hardware detection and heuristics for this CPU | software | 1 |
| ### | PME offload with OpenCL | Enabled PME offload support with OpenCL on NVIDIA and Intel GPUs | A feature that was previously disabled and is now enabled | software | 0 |
| ### | Solaris with GCC | Fixed building on Solaris with GCC | A fix to enable building GROMACS on this OS | software | 2 |
| ### | release tarballs checksum | Provide checksum to validate release tarballs | A new feature to validate the integrity of release tarballs | software | 0 |
| ### | decoupling without SD | Change grompp warning about decoupling without SD to a note | A change in the severity of the message about this simulation setup | software | 1 |
| ### | rerun with no GPU | Calculate Coulomb and LJ reciprocal terms in rerun | A fix for not calculating reciprocal terms in reruns on CPU-only builds | software | 0 |
| ### | Intel compiler errors | Fix compiler errors with Intel compiler | A fix for a compiler error with recent Intel compilers | software | 0 |

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| ### | GPU detection errors | Avoid cryptic GPU detection errors when devices are unavailable or out of memory | A fix for cryptic errors when GPU devices are unavailable | software | 1 |
| ### | uninitialized data on PME only ranks | Fix use of uninitialized data on PME only ranks | A fix for uninitialized PME datastructures when building with clang | software | 1 |
| ### | Apple Clang compiler | Work around broken Apple Clang compiler in Mac OS Catalina | A workaround for a compiler bug related to stack alignment | software | 1 |
| ### | intermolecular interactions and domain decomposition | Fix error with intermolecular interactions and domain decomposition | A fix for an error with long-distance intermolecular interactions and DD | software | 1 |
| ### | AWH initial stage | Remove assertion failure with AWH when not using the initial stage | A fix for an assertion failure when the initial stage is not used | software | 1 |
| ### | gmx angle tool output | Remove problematic output of gmx angle tool | The calculation of standard deviation for empty populations was removed | software | 0 |
| ### | libhwloc headers and runtime | Check that libhwloc headers and runtime match | A fix to prevent mismatches between compile-time and run-time libhwloc versions | software | 1 |
| ### | .gro file formatting | Fix .gro file formatting with large boxes | A fix to ensure proper whitespace separation for large box vectors | data format | 1 |
| ### | PDB CONECT record output | Fix duplicate PDB CONECT record output | A fix to prevent duplicated CONECT records in PDB files | data format | 1 |
| ### | bonded interactions in wrong GPU stream | Fix performance issue with bonded interactions in wrong GPU stream | A fix for a performance issue caused by placing bonded interactions in the wrong GPU stream | software | 1 |
| ### | CMAP across box boundary | Fix incorrect pressure when atoms in CMAP cross a box boundary | A fix for incorrect pressure calculation when a CMAP term spans a periodic boundary | software | 0 |
| ### | LJ cut-off on GPU | Fix incorrect LJ cut-off on GPU when rvdw < rcoulomb | A fix for an incorrect initial LJ cut-off on the GPU in certain scenarios | software | 1 |
| ### | missing bonded forces with CUDA GPUs and DD | Fix (unlikely) missing bonded forces with CUDA GPUs and domain decomposition | A fix for a rare case of missing bonded forces with this setup | software | 0 |
| ### | final kinetic energy and temperature reporting | Fix incorrect reporting of final kinetic energy and temperature | A fix for incorrect reporting of KE and temperature at the last step in certain cases | software | 0 |
| ### | cosine COM pulling | Fix segmentation fault in grompp and mdrun with cosine COM pulling | A fix for a segmentation fault with this feature | software | 1 |
| ### | angle constraints between constraints | Fix grompp not adding angle constraints between constraints | A fix for not replacing bonds with angle constraints when using constraints=all-angles | software | 1 |
| ### | gmx wham with angle and dihedral geometries | Fix gmx wham with angle and dihedral geometries | A fix for an incorrect radian-to-degree conversion | software | 1 |
| ### | gmx xpm2ps library file | Fix bug in gmx xpm2ps | A fix for a failure when no library file was provided | software | 0 |
| ### | gmx anaeig eigenvector reading | Fix bug in gmx anaeig | A fix for an issue when reading a second set of eigenvectors | software | 0 |
| ### | demux.pl script | Fix issue with demux.pl script | A fix for discontinuous trajectories from long replica exchange simulations | software | 1 |
| ### | gmx disre with non-consecutive restraints | Made gmx disre work with non-consecutively labeled restraints | A fix to allow non-consecutive labels for restraints | software | 0 |

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| ### | gro files with index groups | Fixed writing of gro files with index groups | A fix to ensure correct atom name ordering when writing a .gro file from an index group | software | 1 |
| ### | hbond grid | Give meaningful error with too large grid in hbond | A fix to prevent a crash by allocating too much memory for a large grid | software | 0 |
| ### | include delimiters in grompp | Add some information for syntax errors with include delimiters in grompp | Improved error messages for this syntax error | software | 1 |
| ### | reference SIMD setups | Fixed wider reference SIMD setups | A fix for a too-small memory alignment in reference SIMD builds | software | 1 |
| ### | Apple Clang build failure | Fixed build failure with Apple Clang | A fix for a build failure due to qsort being undefined | software | 0 |
| ### | awh1-dim1-period | Removed non-existent mdp option awh1-dim1-period from user guide | Removal of a non-existent option from the documentation | software | 1 |
| ### | pull geometry direction-periodic with AWH | Disallow pull geometry direction-periodic with AWH | A change to disallow this combination to prevent incorrect behavior | identifier | 1 |
| ### | gmx cluster -clndx indices | gmx cluster -clndx indices now correct | A fix for off-by-one errors in the reported cluster indices | software | 1 |
| ### | gmx editconf chain IDs | gmx editconf -f in.pdb -o out.pdb again preserves chain IDs | A fix for an inadvertently broken feature that now preserves chain IDs | software | 0 |
| ### | gmx nmr -viol option | Fix gmx nmr -viol option | A fix for a cryptic error and to enforce exclusivity with other analysis modes | software | 1 |
| | checkpoint restart | Fix checkpoint restart with non-zero initial step | A fix for ignoring the init-step mdp parameter on restart | software | 3 |
| | Colvars active | colvars-active | An mdp option to enable the Colvars module | identifier | 0 |
| | Einstein relation (diffusion) | Einstein relation | A formula that relates the diffusion constant to the mean square displacement | method | 0 |
| | GROMACS simulation runner | gmx mdrun | The main GROMACS program for running simulations | software | 0 |
| | gmxapi.mdrun | gmxapi.mdrun | The gmxapi operation for running a molecular dynamics simulation | software | 13 |
| | gmxapi.mdrun runtime arguments | gmxapi.mdrun accepts arbitrary runtime arguments | A feature to pass arbitrary command-line arguments to mdrun via gmxapi | software | 0 |
| | gromos clustering | gromos | A clustering algorithm based on counting neighbors within a cutoff | algorithm | 0 |
| | Normal Mode Analysis | nm | A method to find vibrational frequencies of a system | method | 17 |
| | Pull enable | pull | An mdp option to turn on pulling | identifier | 0 |
| | Sparc64 HPC-ACE | Sparc64 HPC-ACE | A Fujitsu CPU architecture, a deprecated platform | software | 1 |
| | sPME algorithm | sPME algorithm | The smooth Particle Mesh Ewald algorithm for electrostatics | algorithm | 1 |
| | Reference coordinate | (lambda) | A discrete coordinate coupled to the continuous reaction coordinate in AWH | measure\|state | 3 |
| | Block averaging | block averaging | A method to estimate statistical errors from correlated data | method | 1 |
| | gmx-extract-cluster | gmx-extract-cluster | A GROMACS tool to extract frames belonging to a specific cluster | software | 1 |
| | gmx-energy | gmx-energy | A GROMACS tool to extract and analyze energy terms from a simulation | software | 1 |
| | GROMACS coordinate file | gro | GROMACS file format for atomic coordinates and velocities | data format | 1 |
| | Atom type parameter file | atomtypes.atp | File defining atom types and their properties for pdb2gmx | data format | 1 |
| | Termini database file | n.tdb / c.tdb | Files defining modifications for N- and C-terminal residues | data format | 0 |
| | Combination rule parameter | comb-rule | Parameter specifying the combination rule for non-bonded interactions | identifier | 0 |
| | ATOM record | ATOM | A record in a PDB file for a standard amino acid or nucleotide atom | identifier | 0 |

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| | Pull coordinate type | pull-coord?-type | An mdp option to set the pull type (umbrella, constraint, etc.) | identifier | 2 |
| | Pull coordinate groups | pull-coord?-groups | An mdp option specifying which groups define a pull coordinate | identifier | 0 |
| | Rotation type | rot-type | An mdp parameter to select the type of rotation potential | identifier | 1 |
| | Energy analysis tool | gmx energy | A GROMACS tool for analyzing energy files | software | 0 |
| | Cosine acceleration option | cos-acceleration | An mdp option to apply a cosine-shaped acceleration profile | identifier | 0 |
| | NNPot model file | nnpot-modelfile | An mdp option specifying the path to the trained NNP model | identifier\|data format | 0 |
| | Generalized reaction-field | Generalized reaction-field | A feature that only worked with the removed group scheme | software | 2 |